Simcore Software

Processing Modflow

An Integrated Modeling Environment for the Simulation of Groundwater Flow, Transport and Reactive Processes

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1

Introduction

Processing Modflow (**PM**) was originally developed to support the first official release of MODFLOW-88 [85] to simulate the inundation process of an abandoned open-cast coal mine. Since the release of MODFLOW-88, many computer codes have been developed to add functionalities to MODFLOW or to use MODFLOW as a flow-equation solver for solving specific problems. Consequently, several versions of **PM**[17][22][24] have been released to utilize latest computer codes, to facilitate the modeling process, and to free up modelers from tedious data input for more creative thinking. The computer codes that are supported by present version of Processing Modflow are given in the following section.

1.1 Supported Computer Codes

- MODFLOW [85][54][55][56][63][57]
  MODFLOW is a modular three-dimensional finite-difference groundwater model published by the U. S. Geological Survey. The first public version of MODFLOW was released in 1988 and is referred to as MODFLOW-88. MODFLOW-88 and the later version of MODFLOW-96 [54][55] were originally designed to simulate saturated three-dimensional groundwater flow through porous media. MODFLOW-2000 [56] attempts to incorporate the solution of multiple related equations into a single code. To achieve the goal, the code is divided into entities called processes. Each process deals with a specific equation. For example, the Groundwater Flow Process (GWF) deals with the groundwater-flow equation and replaces the original MODFLOW. The parameter estimation capability of MODFLOW-2000 is implemented by Hill and others [63] using three processes in addition to the GWF process. The Observation Process (OBS) calculates simulated values that are to be compared to measurements, calculates the sum of squared, weighted differences between model values and observations and calculates sensitivities related to the observations. The Sensitivity Process (SEN) solves the sensitivity equation for hydraulic heads throughout the

grid, and the Parameter-Estimation (PES) Process solves the modified Gauss-Newton equation to minimize an objective function to find optimal parameter values. Although the OBS, SEN and PES processes allow MODFLOW-2000 to perform a model calibration without the need for any external parameter estimation software, there will still be many situations in which it is preferable to calibrate a MODFLOW model using external parameter estimation software rather than using built-in MODFLOW-2000 parameter estimation functionality [36]. To combine the strengths of PEST-ASP and MODFLOW-2000, a modified version of MODFLOW-2000, called MODFLOW-ASP [35], allows a coupled PEST-ASP+MODFLOW-2000 approach using MODFLOW-ASP to calculate derivatives and using PEST-ASP to estimate parameter values. The latest major version of MODFLOW was released in 2005, called MODFLOW-2005 [57]. This version, however, does not support parameter estimation process at the time of this writing. As a result, users are encouraged to take advantage of external parameter-estimation programs such as PEST.

- PEST [33][37][38]
  The purpose of PEST is to assist in data interpretation and in parameter estimation. If there are field or laboratory measurements, PEST an adjust model parameters and/or excitation data in order that the discrepancies between the pertinent model-generated numbers and the corresponding measurements are reduced to a minimum. PEST does this by taking control of the model (MODFLOW) and running it as many times as is necessary in order to determine this optimal set of parameters and/or excitations. PEST includes many cutting-edge parameter estimation techniques. According to Doherty [37], the most profound advance is the ”SVD-assist” scheme. This method combines two important regularization methodologies–”truncated singular value decomposition” and ”Tikhonov regularization”.
- MODPATH [93][93][94]
  MODPATH is a particle tracking code written in FORTRAN. To run a particle tracking simulation with MODPATH, the users need to key in parameters in a text screen and have the options to save the input values in a separate file for later use. A graphical post-processor, such as MODPATH-PLOT [95], 3D Groundwater Explorer [21] or 3D Master[23], is required for displaying the calculated pathlines and particle locations.
- PMPATH [19]
  PMPATH is a Windows-based advective transport model for calculating and animating path lines of groundwater. PMPATH uses a semi-analytical particle-tracking scheme used in MODPATH [93] to calculate the groundwater paths and travel times. PMPATH supports both forward and backward particle-tracking schemes for steady-state and transient flow fields. The graphical user interface of PMPATH allows the user to run a particle tracking simulation with just a few clicks of the mouse. Pathlines or flowlines and travel time marks are calculated and displayed along with various on-screen graphical options including head or drawdown contours and velocity vectors.
- MOC3D [74]

MOC3D is a single-species transport model computes changes in concentration of a single dissolved chemical constituent over time that are caused by advective transport, hydrodynamic dispersion (including both mechanical dispersion and diffusion), mixing or dilution from fluid sources, and mathematically simple chemical reactions, including decay and linear sorption represented by a retardation factor. MOC3D uses the method of characteristics to solve the transport equation on the basis of the hydraulic gradients computed with MODFLOW for a given time step. This implementation of the method of characteristics uses particle tracking to represent advective transport and explicit finite-difference methods to calculate the effects of other processes. For improved efficiency, the user can apply MOC3D to a subgrid of the primary MODFLOW grid that is used to solve the flow equation. However, the transport subgrid must have uniform grid spacing along rows and columns. Using MODFLOW as a built-in function, MOC3D can be modified to simulate density-driven flow and transport.

- MT3D [117][120]
  MT3D is a single-species transport model uses a mixed Eulerian-Lagrangian approach to the solution of the three-dimensional advective-dispersive-reactive transport equation. MT3D is based on the assumption that changes in the concentration field will not affect the flow field significantly. This allows the user to construct and calibrate a flow model independently. After a flow simulation is complete, MT3D simulates solute transport by using the calculated hydraulic heads and various flow terms saved by MODFLOW. MT3D can be used to simulate changes in concentration of single species miscible contaminants in groundwater considering advection, dispersion and some simple chemical reactions. The chemical reactions included in the model are limited to equilibrium-controlled linear or non-linear sorption and first-order irreversible decay or biodegradation. Since most developers focus their efforts on supporting its successor MT3DMS [121], MT3D is considered to be obsolete in terms of further development.
- MT3DMS [121][123]
  MT3DMS is a further development of MT3D. The abbreviation MS denotes the Multi-Species structure for accommodating add-on reaction packages. MT3DMS includes three major classes of transport solution techniques, i.e., the finite difference method; the particle tracking based Eulerian-Lagrangian methods; and the higher-order finite-volume TVD method. In addition to the explicit formulation of MT3D, MT3DMS includes an implicit iterative solver based on generalized conjugate gradient (GCG) methods. If this solver is used, dispersion, sink/source, and reaction terms are solved implicitly without any stability constraints.
- MT3D99 [122]
  MT3D99 is an enhanced version of MT3DMS [121] for simulating aerobic and anaerobic reactions between hydrocarbon contaminants and any user-specified electron acceptors, and parent-daughter chain reactions for inorganic or organic compounds. The multi-species reactions are fully integrated with the MT3DMS transport solution schemes, including the implicit solver.
- RT3D [25][26][27] is a code for simulating three-dimensional, multispecies, reactive transport in groundwater. Similar to MT3D99, the code is based on

MT3DMS [121]. MT3D99 and RT3D can accommodate multiple sorbed and aqueous phase species with any reaction framework that the user wishes to define. With the flexibility to insert user-specific kinetics, these two reactive transport models can simulate a multitude of scenarios. For example, natural attenuation processes can be evaluated or an active remediation can be simulated. Simulations could potentially be applied to scenarios involving contaminants such as heavy metals, explosives, petroleum hydrocarbons, and/or chlorinated solvents.

- PHT3D [96][97]
  PHT3D couples MT3DMS [123] for the simulation of three-dimensional advective-dispersive multi-component transport and the geochemical model PHREEQC-2 [91] for the quantification of reactive processes. PHREEQC-2, in its original version, is a computer program written in the C programming language that is designed to perform a wide variety of low-temperature aqueous geochemical calculations. PHT3D uses PHREEQC-2 database files to define equilibrium and kinetic (e.g., biodegradation) reactions. For the reaction step, PHT3D simulations might include (1) Equilibrium complexation reaction/speciation within the aqueous phase, (1) Kinetically controlled reactions within the aqueous phase such as biodegradation, (3) Equilibrium dissolution and precipitation of minerals, (4) Kinetic dissolution and precipitation of minerals, (5) Single or multi-site cation exchange (equilibrium), and (6) Single or multi-site surface complexation reactions.
- SEAWAT [51][76][77]
  SEAWAT is designed to simulate three-dimensional, variable-density, saturated groundwater flow and transport. The original SEAWAT program was developed by Guo and Langevin [51] based on MODFLOW-88 and an earlier version of MT3DMS [121]. The program has subsequently been modified to couple MODFLOW-2000 [56] and a later version of MT3DMS [123]. Flexible equations were added to the fourth version of the program (i,e., SEAWAT_V4 [77]) to allow fluid density to be calculated as a function of one or more MT3DMS species. Fluid density may also be calculated as a function of fluid pressure. The effect of fluid viscosity variations on groundwater flow was included as an option. This option is, however, not supported by **PM**. Although MT3DMS and SEAWAT are not explicitly designed to simulate heat transport, temperature can be simulated as one of the species by entering appropriate transport coefficients. For example, the process of heat conduction is mathematically analogous to Fickian diffusion. Heat conduction can be represented in SEAWAT by assigning a thermal diffusivity for the temperature species (instead of a molecular diffusion coefficient for a solute species). Heat exchange with the solid matrix can be treated in a similar manner by using the mathematically equivalent process of solute sorption. See Langevin and others [77] for details about heat transport.
- Water Budget Calculator [18]: This code calculates the groundwater budget of user-specified subregions and the exchange of flows between subregions.

1.2 Compatibility Issues

For many good reasons, MODFLOW and most of its related groundwater simulation programs, such as MT3DMS, are written in FORTRAN and save simulation results in binary files. This includes groundwater models distributed by the U. S. Geological Survey and most popular graphical user interfaces, such as Processing Modflow, ModIME [119], Groundwater Modeling System (known as GMS), Groundwater Vistas, Argus ONE, and Visual MODFLOW. **PM** is capable of reading binary files created by the above-mentioned codes.

Binary files are often saved in the "unformatted sequential" or "transparent" format. An unformatted sequential file contains record markers before and after each record, whereas a transparent file contains only a stream of bytes and does not contain any record markers. Of particular importance is that different FORTRAN compilers often use different (and incompatible) formats for saving "unformatted sequential" files. Thus, when compiling your own codes the following rules should be followed, so that **PM** can read the model generated binary files.

- When Lahey Fortran compiler is used:
  - Create a transparent file by specifying FORM = 'UNFORMATTED' and ACCESS = 'TRANSPARENT' in the OPEN statement.
- When Intel Visual Fortran is used:
  - Create a transparent file, if it is opened using FORM = 'BINARY' and ACCESS = 'SEQUENTIAL'.
- If you are using other compilers, please consult the user manual for the settings of creating "transparent" binary files.

2

Modeling Environment

This chapter is a complete reference of the user interface of **PM**.

With the exception of PHT3D, **PM** requires the use of consistent units throughout the modeling process. For example, if you are using length $[L]$ units of meters and time $[T]$ units of seconds, hydraulic conductivity will be expressed in units of $[m/s]$, pumping rates will be in units of $[m^3/s]$ and dispersivity will be in units of $[m]$. The values of the simulation results are also expressed in the same units. Table 2.1 lists symbols and their units, which are used in various parts of this text.

PHT3D requires the use of meters for the length, the use of mol/l_w for concentrations of aqueous (mobile) chemicals and user-defined immobile entities such as bacteria and the use of mol/l_v for mineral, exchanger and surface concentrations, where mol refers to moles, l_w refers to liter of pore water and l_v refers to liter of bulk volume (see Prommer and others [97] for details about the use of units in PHT3D).

PM contains the following menus *File*, *Grid*, *Parameters*, *Models*, *Tools*, *Value*, *Options*, and *Help*. The *Value* and *Options* menus are available only in the Grid Editor and Data Editor (see Sections 2.1 and 2.2 for details). **PM** uses an intelligent

Table 2.1 Symbols used in the present text

Symbol	Meaning	Unit
m	thickness of a model layer	$[L]$
HK	horizontal hydraulic conductivity along model rows	$[LT^{-1}]$
VK	vertical hydraulic conductivity	$[LT^{-1}]$
T	transmissivity; T = HK $\times$ m	$[L^2T^{-1}]$
S_s	specific storage	$[L^{-1}]$
S	storage coefficient or storativity; S = Ss $\times$ m	$[-]$
S_y	specific yield or drainable porosity	$[-]$
n_e	effective porosity	$[-]$
$VCONT$	vertical leakance	$[T^{-1}]$
$HANI$	horizontal anisotropy	$[-]$
	$HANI \times HK$ = horizontal hydraulic conductivity along columns	
$VANI$	vertical anisotropy; $HK = VK \times VANI$	$[-]$

Table 2.2 Summary of menus in **PM**

Menu	Description
File	Create new models; open existing models; convert models to the **PM** format; Save and print plots.
Grid	Generate or modify the size of a model grid; input of the geometry of the aquifer.
Parameters	Input of spatial aquifer parameters, for example transmissivity; Input of temporal parameters, for example simulation length or number of stress periods.
Models	Specify model-specific data using the module provided and call simulation programs. For example, the user can add wells, use the recharge or river modules to MODFLOW or define the advection or dispersion parameters in MT3DMS. The simulation programs are called by selecting Run from the corresponding model.
Tools	Call the modeling tools.
Value	Manipulate model data; read or save model data in separate files; import model results; import an existing MODFLOW input file.
Options	Modify the appearance of the model grid on the screen; load site maps; change display mode; change input method.
Help	Call Processing Modflow Pro Help.

menu system to help you control the modeling process. If a model data set has been specified, the corresponding item of the *Grid*, *Parameters*, and *Models* menus will be checked. To deactivate a selected item in the Models menu, just select the item again. If the user does not know which model data still needs to be specified, one may try to run the model by selecting the menu item *Run* from the corresponding model in the *Models* menu. **PM** will check the model data prior to running the model. A summary of the menus in **PM** is given in Table 2.2.

A toolbar with buttons representing **PM** operations or commands is displayed below the menus. The toolbar is a shortcut for the pull-down menus. To execute one of these shortcuts, move the mouse pointer over the toolbar button and click on it.

Most of the user-specified data is saved in binary files. Prior to running the supported models or the parameter estimation programs, **PM** will generate the required ASCII input files. The names of the ASCII input files are given in Section 6.3. The formats of the input files of can be found in the user's guides of the corresponding model. The particle-tracking model PMPATH retrieves the binary data files of **PM** directly, thus no ASCII input file is required by PMPATH.

2.1 The Grid Editor

The first steps in the groundwater modeling process are to define the goals of the model, select a computer code, collect the necessary data, develop a conceptual model of the groundwater system and define the spatial discretization of the model domain. Anderson and Woessner [8] discuss the steps in going from aquifer systems to a numerical model grid. Zheng and Bennett [118] describe the design of

model grids, which are intended for use both in flow and transport simulations. These sources provide valuable general information relating to spatial discretization and grid design in numerical groundwater modeling.

In the block-centered finite difference method, an aquifer system is replaced by a discretized domain consisting of an array of nodes and associated finite difference blocks (cells). Fig. 2.1 shows the spatial discretization scheme of an aquifer system with a mesh of cells and nodes at which hydraulic heads are calculated. The nodal grid forms the framework of the numerical model. Hydrostratigraphic units can be represented by one or more model layers. The thickness of each model cell and the width of each column and row can be specified. The locations of cells are described in terms of layers, rows, and columns. **PM** uses an index notation [Layer, Row, Column] for locating the cells. For example, the cell located in the first layer, 6th row, and 2nd column is denoted by [1, 6, 2]. To generate or modify a model grid, select *Grid* |

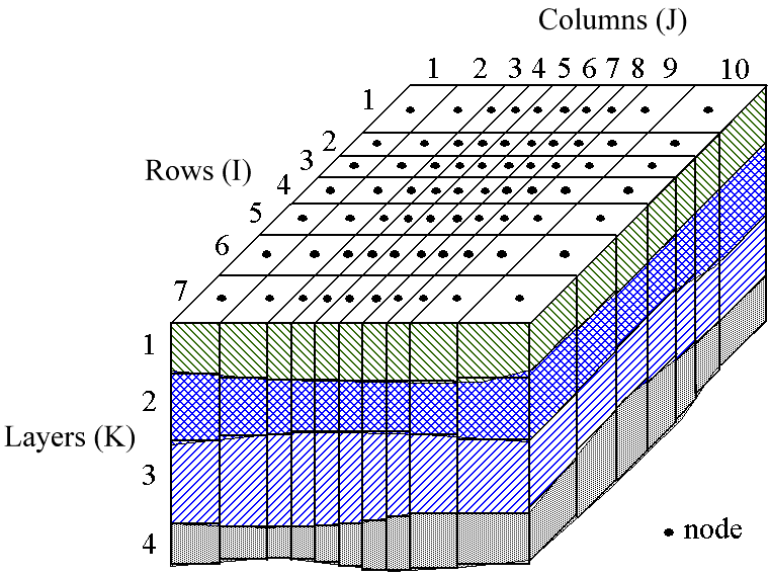


Fig. 2.1. Spatial discretization of an aquifer system and the cell incides

Mesh Size. If a grid does not exist, a Model Dimension dialog box (Fig. 2.2) appears for specifying the extent and number of layers, rows, and columns of the model grid. After specifying these data and clicking the *OK* button, the Grid Editor shows the model grid (Fig. 2.3). A summary of the tool bar buttons of the Grid Editor is given in Table 2.3. Using the Environment Options dialog box (see Section 2.9.2), the user can adjust the coordinate system, the extent of the Viewing Window and the position of the model grid to fit the study site. By default, the origin of the coordinate system is set at the lower-left corner of the model grid and the extent of the Viewing Window is set to twice that of the model grid. The first time the Grid Editor is used, the user

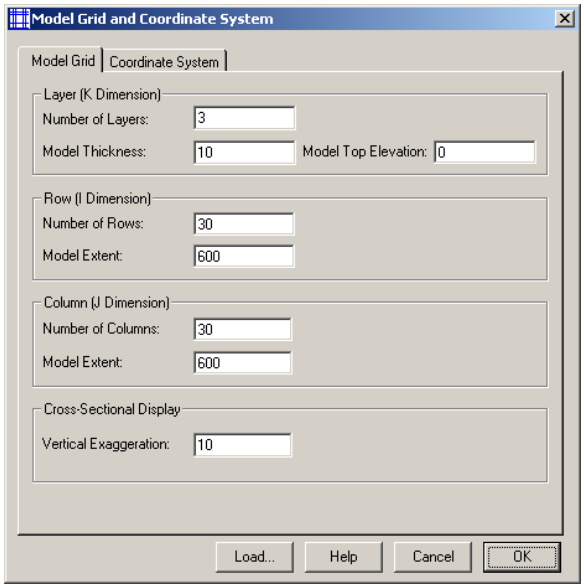


Fig. 2.2. The Model Dimension dialog box

can insert or delete columns or rows (see below). After leaving the Grid Editor and saving the grid, the existing model grid can be subsequently refined by calling the Grid Editor again. In each case, the width of any column or row can be modified. If the grid is refined, depending on the nature of the model parameters, they are either kept the same or scaled by the cell size. The following rules apply:

1. Pumping rates, mass-loading rate (see Section 2.6.2.9) and cell-by-cell conductance values of the river, drain, general-head boundary, and stream are scaled by the cell volume. For example, if a well cell is refined to four cells, all four refined cells will be treated as wells, each with 1/4 of the original pumping rate. The sum of their pumping rates remain the same as that of the previous single well.
2. The parameters of polylines, which are used to define river, drain, general-head boundary, or stream, remain the same, since they are grid-independent. If a stream (of the Stream-Routing package) is defined by using cell-by-cell values, you must redefine the segment and reach number of the stream.
3. Transmissivity (T) and storage coefficient (S) values are scaled by the thickness.
4. All other model parameters remain the same.

► To change the width of a column and/or a row

1. Click the assign value button +.
   The grid cursor appears only if the Assign Value button is pressed down. You do not need to click this button, if it is already depressed.

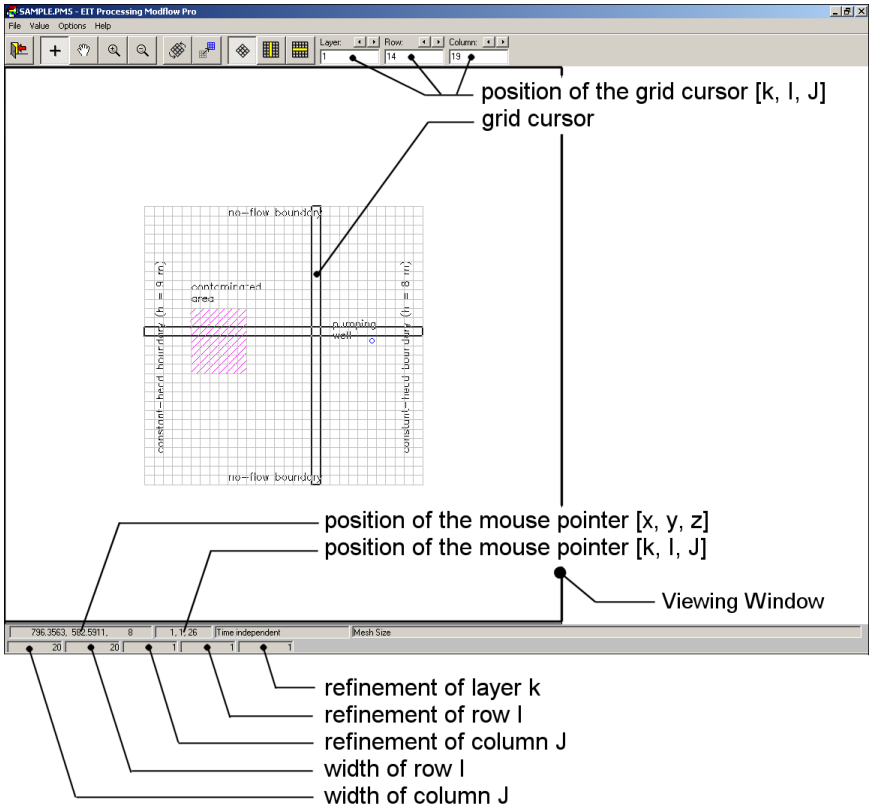

position of the grid cursor [k, I, J]
grid cursor
position of the mouse pointer [x, y, z]
position of the mouse pointer [k, I, J]
Viewing Window
refinement of layer k
refinement of row I
refinement of column J
width of row I
width of column J

Fig. 2.3. The Grid Editor

2. Move the grid cursor to the desired cell by using the arrow keys or by clicking the mouse on the desired position. The sizes of the current column and row are shown on the status bar.
3. Press the right mouse button once. The Grid Editor shows the Grid Size dialog box (Fig. 2.4).
4. In the dialog box, type new values, then click OK.

► To insert or delete a column and/or a row

1. Inserting or deleting columns/rows is only possible when using the Grid Editor for the first time. Click the assign value button +.
2. Move the grid cursor to the desired cell by using the arrow keys or by clicking the mouse on the desired position.
3. Hold down the Ctrl-key and press the up or right arrow keys to insert a row or a column; press the down or left arrow keys to delete the current row or column.

Table 2.3 Summary of the toolbar buttons of the Grid Editor

Button	Name	Action
	Leave editor	Leave the Grid Editor and return to the main menu of **PM**.
	Assign value	Allows the user to move the grid cursor and change the widths of grid columns and rows.
	Pan	Moves the Viewing Window up, down, or sideways to display areas of the model domain which, at the current viewing scale, lie outside the Viewing Window. By dragging the mouse, the model grid and sitemaps will be moved in the same direction as the mouse cursor. When the left mouse button is released, the grid and maps will be redrawn.
	Zoom in	Allows the user to zoom-in by dragging a window over a part of the model domain.
	Zoom out	Display the entire worksheet.
	Rotate grid	To rotate the model grid, point the mouse pointer to the grid, left click and hold down the mouse button, and move the mouse.
	Shift grid	Allows the user to move the model grid to another position. To shift the model grid, point the mouse pointer to the grid, left click and hold down the mouse button, and move the mouse.
	Map View	Switch to the Map View display mode.
	Column View	Switch to the column cross-sectional display mode.
	Row View	Switch to the row cross-sectional display mode.
	Duplication on/off	If duplication is turned on, the size of the current row or column will be copied to all rows or columns passed by the grid cursor. Duplication is on, when this button is depressed.

► To refine a layer, a row or a column

1. Refining a grid is only possible when the grid has already been saved. Click the assign value button .
2. Move the grid cursor to the desired cell by using the arrow keys or by clicking the mouse on the desired position.
3. Press the right mouse button once. The Grid Editor shows the Grid Size dialog box (Fig. 2.4).
4. In the dialog box, type new values, then click OK.

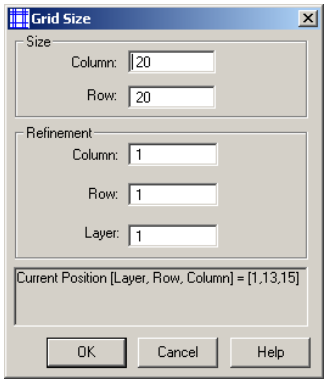


Fig. 2.4. The Grid Size dialog box

2.2 The Data Editor

The Data Editor is used to assign parameter values to the model. To start the Data Editor, select a corresponding item from the *Grid*, *Parameters* or *Models* menus. For example, select *Parameters* | *Porosity* to assign porosity values to the model.

The Data Editor provides four *display mode*s - Map View, Grid View, Column View, and Row View. It has three methods for specifying parameter values - Cell-by-cell, Polygon, and Polyline methods. The *input methods* are discussed in sections 2.2.1, 2.2.2, and 2.2.3. The Polyline method is available only for specifying data to the River, Drain, General-head boundary and Streamflow-Routing packages.

In the Grid View display mode, the Viewing Window is aligned with the model grid (Fig. 2.5). In the Map View display mode, the Viewing Window is aligned with the orthogonal Northing and Easting coordinate axes. A rotated model grid is displayed on the Map View similar to Fig. 2.6. In the Row or Column (cross-sectional) View, the Viewing Window is aligned with the vertical axis (Fig. 2.7).

Using the Environment Options dialog box (see Section 2.9.2) the user can adjust the vertical exaggeration factor for the cross-sectional display, the coordinate system, the horizontal extent of the Viewing Window, and the position of the model grid to fit the condition of the study area. Regardless of the display modes, the mouse pointer position [x, y, z] is always expressed in the *world* coordinates according to the user-defined coordinate system, and [K, I, J] is expressed in [Layer, Row, Column] cell indices. The position of the grid cursor is shown in the tool bar. The grid cursor can be moved by using the arrow keys, clicking the mouse on the desired position, using buttons in the tool bar, or typing the new position in the layer/row/column edit fields and pressing the Enter key. The parameter values of the cell pointed to by the grid cursor are displayed from left to right in the status bar. A summary of the tool bar buttons of the Data Editor is given in Table 2.4.

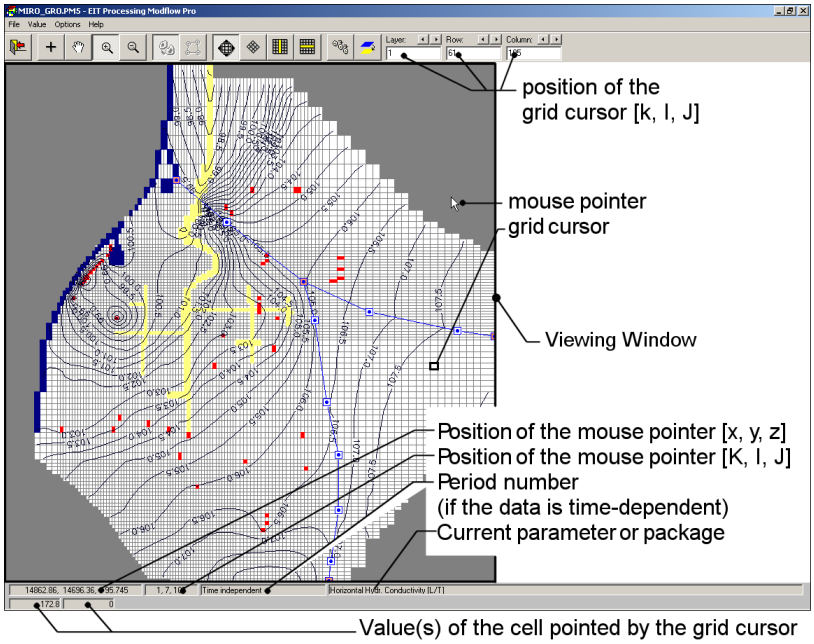

position of the
grid cursor [k, I, J]
mouse pointer
grid cursor
Viewing Window
Position of the mouse pointer [x, y, z]
Position of the mouse pointer [K, I, J]
Period number
(if the data is time-dependent)
Current parameter or package
Value(s) of the cell pointed by the grid cursor

Fig. 2.5. The Data Editor (Grid View)

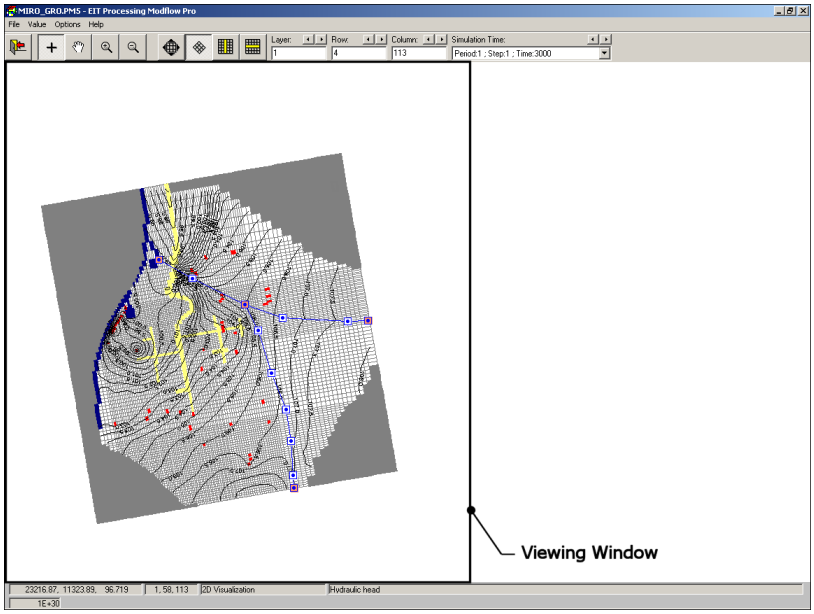


Fig. 2.6. The Data Editor (Map View)

Table 2.4 Summary of the toolbar buttons of the Data Editor

Button	Name	Action
	Leave editor	Leave the Data Editor and return to the main menu.
	Assign value	Allow the user to move the grid cursor and assign values to model cells.
	Pan	Moves the Viewing Window up, down, or sideways to display areas of the model domain which, at the current viewing scale, lie outside the Viewing Window. By dragging the mouse, the model grid and sitemaps will be moved in the same direction as the mouse cursor. When the left mouse button is released, the grid and maps will be redrawn.
	Zoom in	Allow the user to drag a zoom-window over a part of the model domain.
	Zoom out	Display the entire worksheet.
	Cell-by-cell input method	Switch to the Cell-by-cell input method.
	Polygon input method	Switch to the Zone input method.
	Polyline input method	Switch to the Polyline input method.
	Grid view	Switch to the Grid View display mode.
	Map view	Switch to the Map View display mode.
	Column View	Switch to the column cross-sectional display mode.
	Row View	Switch to the row cross-sectional display mode.
	Duplication on/off	If duplication is turned on, the size of the current row or column will be copied to all rows or columns passed by the grid cursor. Duplication is on, when this button is depressed.
	Layer, Row, Column Copy on/off	When this button is depressed, Layer/row/column copy is on and the following rules apply: (1) If the display mode is Grid View or Map View, when moving to another layer the zones and cell values of the current layer will be copied to the destination layer; (2) If the display mode is Row View, when moving to another column the cell values of the current row cross-section will be copied to the destination row cross-section; (3) If the display mode is Column View, when moving to another column the cell values of the current column cross-section will be copied to the destination column cross-section.
	Change stress period	Manage model data for transient simulations.

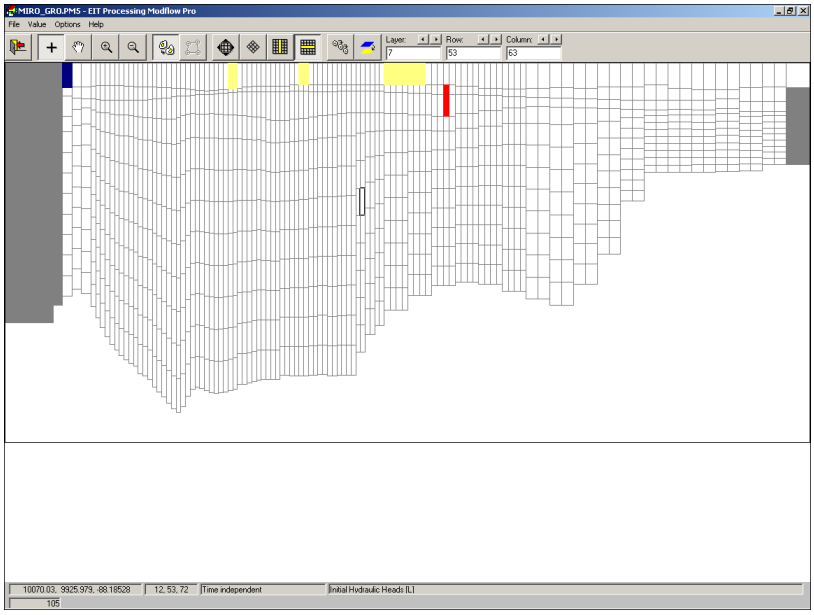


Fig. 2.7. The Data Editor (Cross-sectional View)

2.2.1 The Cell-by-Cell Input Method

To activate this method, click the button or select *Options* | *Input Method* | *Cell-By-Cell*.

► To assign new value(s) to a cell

1. Click the assign value button .
   It is not necessary to click this button, if the button is already depressed.
2. Move the grid cursor to the desired cell by using the arrow keys or by clicking the mouse on the cell. The value(s) of the current cell is (are) displayed in the status bar.
3. Press the Enter key or press the right mouse button once.
   The Data Editor shows a dialog box.
4. In the dialog box, type new value(s) then click OK.

Since groundwater model data are often very complex, **PM** provides several possibilities for checking or modifying cell-by-cell model data as listed below.

- Double-click a cell.
  All model cells with the same value will appear in the same color. The color can be changed by repeated double-clicks.

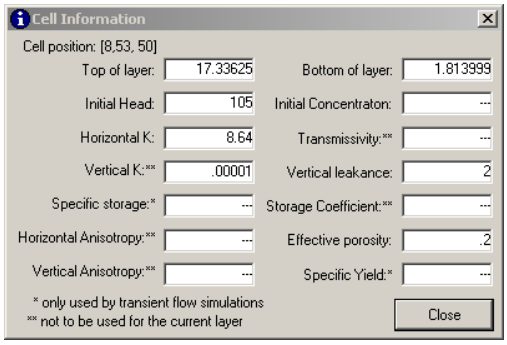


Fig. 2.8. The Cell Information dialog box

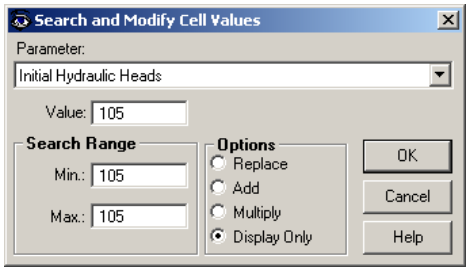


Fig. 2.9. The Search and Modify Cell Values dialog box

- Shift + left mouse button or Ctrl+Q.
  Open the Cell Information dialog box (Fig. 2.8), which displays the user-specified data of the cell pointed to by the grid cursor.
- Ctrl + left mouse button. Open the Search and Modify Cell Values dialog box (Fig. 2.9). This allows you to display all cells that have a value located within the Search Range (to be specified). According to the user specified Value and the operation Options, you can easily modify the cell values. For example, if Add is used, the user-specified value will be added to the cell value. The Parameter drop-down box shows the available parameter type(s). The user may select the parameter to which the subsequent Search and Modify operation will be applied.
- Select *Value* | *Search and Modify* or press Ctrl+S.
  Open a Search and Modify dialog box for more advanced data manipulation features. See Section 2.8.5 for details.

2.2.2 The Polygon Input Method

The Polygon Input Method allows the user to assign parameter values to model cells with the help of polygons. This input method is not allowed in the cross-sectional view. To activate this method, click on the button or the button to switch to Grid View or Map View, and then click on the button or choose *Options* | *Input*

Method | *Polygon*. The use of this input method is straightforward. First, you draw a polygon and then assign parameter values to the polygon. Finally, press the ›› button to apply the parameter values to model cells that lie within the polygon.

Note. Polygon data is not used by PM for model computation directly. If polygon data is not applied to the model cells, the original values in the cells are used.

► To draw a polygon

1. If the display mode is not Grid View or Map View, click the button or the button to switch to the Grid View or Map View.
2. Click the assign value button and click the button.
3. Click the mouse pointer on a desired position to anchor one end of a line.
4. Move the mouse pointer to another position then press the left mouse button again.
5. Repeat steps 3 and 4 until the polygon is closed or press the right mouse button to abort.

► To delete a polygon

1. If the display mode is not Grid View or Map View, click the button or the button to switch to the Grid View or Map View.
2. Click the assign value button and click the button.
3. Move the mouse pointer into a polygon.
   The boundary of the polygon will be highlighted.
4. Press the Delete key.

► To assign value(s) to polygons

1. If the display mode is not Grid View or Map View, click the button or the button to switch to the Grid View or Map View.
2. Click the assign value button and click the button.
3. Move the mouse pointer into a polygon.
   The boundary of the polygon will be highlighted. The value(s) of the polygon will be displayed in the status bar.
4. Press the right mouse button once.
   The Data Editor displays a dialog box, which allows the user to assign parameter value(s) to the polygon.
5. In the dialog box, type new parameter value(s) then click the ›› button to apply the parameter value(s) to the model cells within the polygon.

► **To modify a polygon**

1. The user may drag vertices of a polygon by pointing the mouse pointer at a vertex node and pressing down the left mouse button while moving the mouse.
2. If there are several polygons, some polygons can intersect or even cover other polygons. If the mouse pointer is moved into a covered polygon, the boundary of the polygon will not be highlighted. In this case, simply move the mouse pointer into that polygon, hold down the Ctrl key and press the left mouse button once. The Data Editor will resort the order of the polygons and the ”lost” polygon will be recovered.

2.2.3 The Polyline Input Method

The Polyline Input Method is available only for the Drain, General-head boundary, River and Streamflow-Routing packages. This input method is not allowed in the cross-sectional view. To activate this method, click on the button or the button to switch to Grid View or Map View, and then click on the button or choose *Options* | *Input Method* | *Polyline*. The use of this input method is straightforward. First, you draw a polyline along a drain, river, or stream, and then assign parameter values to vertices of the polyline. Within a polyline, parameter values needed for constructing MODFLOW input files are assigned to at least one vertex. Properties needed for cells along traces of polylines are obtained using the parameter values of vertices. These property values are used in addition to the cell-by-cell values to generate MODFLOW input files prior to running MODFLOW.

► **To draw a polyline**

1. If the display mode is not Grid View or Map View, click the button or the button to switch to the Grid View or Map View.
2. Click the assign value button and click the button.
3. Click the mouse pointer on a desired position to anchor one end of a line.
4. Move the mouse pointer to another position then press the left mouse button again.
5. Repeat steps 3 and 4 until the desired polyline is drawn, click on the latest vertex again to complete the polyline or press the right mouse button to abort drawing.

► **To delete a polyline**

1. If the display mode is not Grid View or Map View, click the button or the button to switch to the Grid View or Map View.
2. Click the assign value button .
3. Move the mouse pointer over a polyline. The polyline will be highlighted.
4. Press the Delete key.

Follow the steps below to assign parameter values to polylines. Refer to the explanation of the River, Drain, General-head boundary, and Streamflow-routing packages for details about the required parameters of each package.

► **To assign value(s) to polylines**

1. If the display mode is not Grid View or Map View, click the button or the button to switch to the Grid View or Map View.
2. Click the assign value button and click the button.
3. Move the mouse pointer over a vertex and right-click.
   The Data Editor displays a dialog box, which allows the user to assign parameter value(s) to the vertex.
4. In the dialog box, type new parameter value(s).
   Once the parameter values are specified, the display color of the vertex is changed to indicate that its parameter values are specified.

► **To modify a polyline**

1. The user may drag vertices of a polyline by pointing the mouse pointer at a vertex node, pressing down the left mouse button, and moving the mouse.
2. Use Shift+left click on a segment of the polyline to insert a new vertex.
3. Use ctrl+left click on a vertex to delete it.

2.2.4 Specifying Data for Transient Simulations

If a model has more than one stress period, the button appears in the Tool bar. Clicking on this button opens the Temporal Data dialog box (Fig. 2.10), which is used to manage model data for transient simulations. The following describes the use of the dialog box.

- The table displays the status of the model data of each stress period. The boxes in the Data Status column have three states:
  - ☒: Model data has been specified and will be used for the simulation.
  - ☐: Model data has been specified, but will not be used. The model data from the previous stress period will be used for the simulation.
  - ☐: Model data has not been specified. The model data from the previous stress period will be used for the simulation.

  Click on the Data boxes to toggle between ☒ and ☐. Fig. 2.10 shows an example in which the model data for the periods 1, 3, 4 are specified. The specified data of the first period will be used throughout the first three periods. The data of the fourth period will be used for the rest of the simulation. The model data of the third period has been specified, but will not be used for the simulation since the Data Status is ☐.

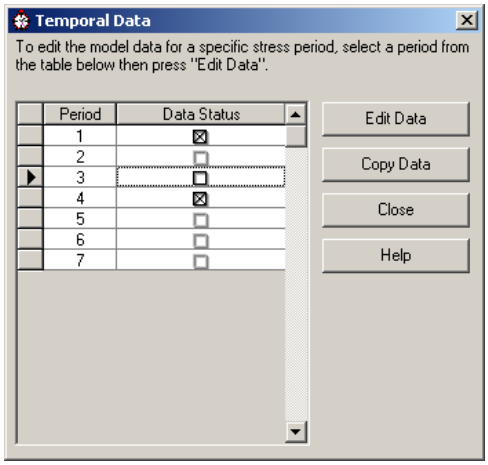


Fig. 2.10. The Temporal Data dialog box

- Edit Data: To edit model data for a particular stress period, select a row of the table and click the Edit Data button. After having specified the model data of a stress period, the Data status changes to ☒.
- Copy Data: To copy model data from one stress period to another.

2.3 The File Menu

2.3.1 New Model

Select New Model to create a new model. A New Model dialog box allows the user to specify a filename on any available folder or drive for the new model. A **PM** model must always have the file extension .pm5, which has been kept consistent since PMWIN version 5. All file names valid under the MS Windows operating system with up to 120 characters can be used. It is a good idea to save every model in a separate folder, where the model and its output data will be kept. This will also allow the user to run several models simultaneously (multitasking).

2.3.2 Open Model

Use Open Model to load an existing **PM** model. Once a model is opened, **PM** displays the filename of the model on the title bar.

2.3.3 Convert Model

A Convert Models dialog box appears after selecting this menu item. The options in this dialog box are grouped under 4 tabs - PMWIN 4.x, MODFLOW-88/96,

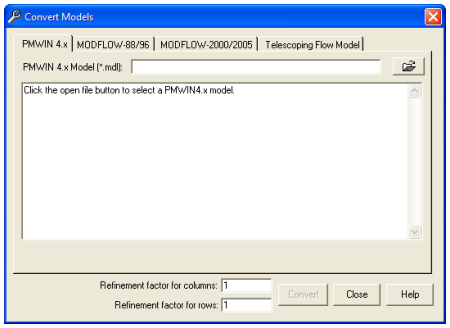


Fig. 2.11. The Convert Model dialog box

MODFLOW-2000/2005, and Telescoping Flow Model (Fig. 2.11). The tabs are described below. In addition, the user can specify refinement factors for both column and row directions. In this way, one can load or create a model with a higher resolution for transport simulations.

- PMWIN 4.x tab: This tab is used to convert groundwater models created by PMWIN 4.x to **PM**. To convert, click the open file button and select a PMWIN 4.x model from an Open dialog box, then click the Convert button to start the conversion. Groundwater models created by PMWIN 5.x or later are compatible with **PM** and do not need to be converted.
- MODFLOW-88/96 tab: This tab is used to import models stored in MODFLOW-88 or MODFLOW-96 formats to **PM**. To import, click the open file button and select a MODFLOW Name File from an Open dialog box, then click the Convert button to start the conversion. Refer to Section 6.3.1 for the definition of the name file. A MODFLOW-88/96 name file usually has lines with the file type (i.e., Ftype) ”BAS” or ”BCF”.
- MODFLOW-2000/2005 tab: This tab is used to import models stored in MODFLOW-2000/2005 formats to **PM**. To import, click the open file button and select a MODFLOW Name File from an Open dialog box, then click the Convert button to start the conversion. Refer to Section 6.3.1 for the definition of the name file. A MODFLOW-2000/2005 name file usually has lines with the file type (i.e., Ftype) ”BAS6”, ”BCF6”, or ”LPF”.
- Telescoping Flow Model (Fig. 2.12): This tab creates local-scale sub-models from a regional scale model. To create a sub-model, select an existing **PM** model and specify the sub-region. Then click the Convert button. Prior to converting, the flow simulation of existing **PM** model must be performed. The sub-region is defined by the starting and ending columns and rows. **PM** automatically transfers the model parameters and the calculated heads from the regional model to the sub-model. The boundary of the sub-model will be set to constant head boundary (for steady-state simulations) or time-variant specified-head boundary (for transient simulations).

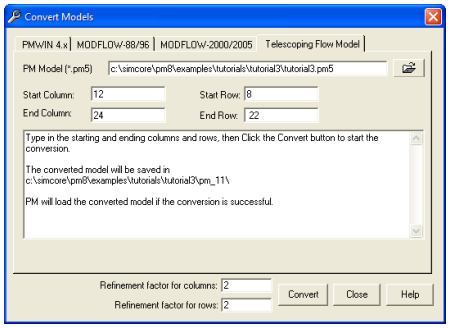


Fig. 2.12. Telescoping a flow model using the Convert Model dialog box

2.3.4 Preferences

The Preferences dialog box (Fig. 2.13) defines the MODFLOW version and manages the paths to the simulation programs of an opened **PM** model. The settings of the dialog box are described below.

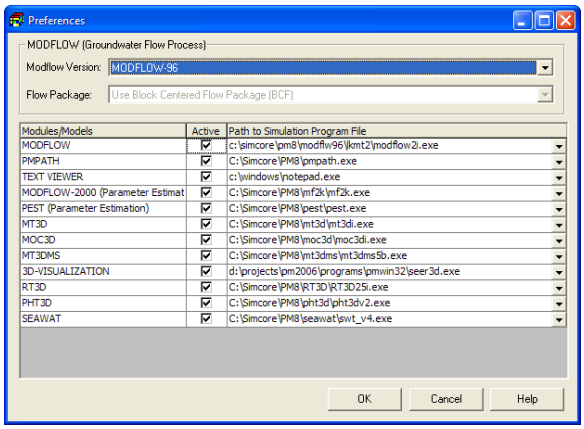


Fig. 2.13. The Preferences dialog box

- *Modflow Version*: Several variants of MODFLOW are supported and included in **PM**. Each variant is associated with an executable program. The full paths and file names of all executable programs of MODFLOW are given in Table 2.5. The default Modflow Version is ”MODFLOW-96”. This version works with all supported transport models. Of particular note is that when using MODFLOW-2000 for parameter estimation, *Modflow Version* must be set to ”MODFLOW-2000/MODFLOW-2005”, otherwise it is not possible to switch the Flow Package (see below) to the LPF package, which are required for estimating aquifer parameters within MODFLOW-2000.

- *Flow Package*: This dropdown box is enabled, when *Modflow Version* is set to MODFLOW-2000/MODFLOW-2005, which includes the Layer-Property Flow (LPF) and the Block-Centered Flow (BCF) packages for formulating inter-cell hydraulic conductance terms. As the BCF or LPF packages require different aquifer parameters for formulating finite difference equations of groundwater flow, it is important to notice the following major differences between these two packages:
  - The Block Centered Flow (BCF) package supports four layer types. Depend on the selected layer type; the required aquifer parameters of a model layer are different and listed below. Layer type 0: T and S
    Layer type 1: HK and Sy.
    Layer type 2: T, S and Sy.
    Layer type 3: HK, Sy and S.
    Note that S and Sy are required only for a transient flow simulation. All layer types use VCONT to describe the vertical conductance between two layers.
  - The Layer-Property Flow package has only two layer types - confined and convertible (i.e., convertible between confined and unconfined). Independent of the selected layer type; a model layer always requires HK, Ss, and VK or VANI. The only exception is Sy, which is required only if the layer is convertible (note that Ss and Sy are required only for a transient flow simulation). When the Layer-Property Flow package is selected, the menu items Transmissivity, Vertical Leakance and Storage Coefficient of the Parameters menu are dimmed and cannot be used (don't need to be used).

  Note.
  - All versions of Modflow and either BCF or LFP package can be used with PEST for estimating parameters. However, one can only estimate the required aquifer parameters of the BCF or LPF package as given above.
  - As the BCF package does the not support the required parameterization method of MODFLOW-2000, this package cannot be used with the built-in model calibration capability of MODFLOW-2000. That is, the user cannot estimate aquifer parameters when using BCF with MODFLOW-2000.
  - The settings of Modflow Version and Flow Package are saved with the model, i.e., if the model is used on another computer these settings will remain the same.

Table 2.5 Versions and Filenames of MODFLOW

Version	Filename
MODFLOW-96	pmdir\modflw96\lkmt2\modflow2i.exe
MODFLOW-2000	pmdir\mf2k\mf2ki.exe
MODFLOW-2005	pmdir\modflow2005\mf2005.exe

– pmdir is the folder in which **PM** is installed, for example C:\Simcore\PM8.

- *Module/Models*: The supported modules or models are listed below. Each module/model is associated with a program. Note that some modules are optional and may not appear on the user's computer.
  - *MODFLOW* is groundwater flow simulation program, which is used when selecting the menu item *Modflow* | *Run*.
  - *PMPATH* is a particle-tracking model (also referred to as advective transport) included in **PM**.
  - *Text Viewer*, which can be any text editors, is used to display simulation result files, which are saved in ASCII.
  - *MODFLOW-2000 (Parameter Estimation)*: The associated program is used when selecting the menu item *MODFLOW-2000 (Parameter Estimation)* | *Run* | *MODFLOW-2000*.
  - *PEST (Parameter Estimation)*: PEST [33][34] is a program for parameter estimation. The associated program is used when selecting the menu item *PEST (Parameter Estimation)* | *Run* or *MODFLOW-2000 (Parameter Estimation)* | *Run* | *PEST-ASP+MODFLOW-2000*. Note that the latter requires PEST-ASP and a special version of MODFLOW-2000, called MF2K-ASP, which are automatically installed.
  - *MT3D*: MT3D is a single-species solute transport model, which has been prepared by Zheng [117][120] and has been improved subsequently over years. The associated program is used when selecting the menu item MT3D | Run.
  - *MOC3D*: MOC3D [74] is a single-species solute transport model using the method of characteristics. The associated program is used when selecting the menu item *MOC3D* | *Run*.
  - *MT3DMS*: MT3DMS [121][123] is a multi-species solute transport model. The associated program is used when selecting the menu item *MT3DMS/SEAWAT* | *Run*. If the user intends to use MT3D99 [122], the MT3D99 program should be assigned to this module, and the MT3D99 and MODFLOW programs must be compiled with the same compiler.
  - *3D Visualization*: The software Seer3D [] is available separately. When installed, Seer3D can be started by selecting the menu item *Tools* | *3D Visualization*.
  - *RT3D*: The RT3D model [25][26][27]) simulates reactive-flow and transport of multiple mobile and/or immobile species. The **PM** installation includes three versions of RT3D - rt3d1v.exe (version 1), rt3d2v.exe (version 2), and rt3d25v.exe (version 2.5). They can be found in the folder \pmhome\rt3d, where pmhome is the installation directory of **PM**. The associated program is used when selecting the menu item *RT3D* | *Run*.
  - *PHT3D*: PHT3D [97] couples MT3DMS [123] for the simulation of three-dimensional advective-dispersive multi-component transport and the geochemical model PHREEQC-2 [91] for the quantification of reactive processes. The associated program is used when selecting the menu item *PHT3D* | *Run*.

  - *SEAWAT*: SEAWAT is designed to simulate three-dimensional, variable-density, saturated groundwater flow and transport. The associated program is used when selecting the menu item *MT3DMS/SEAWAT | Run*.
- *Active*: Check or clear the active flag to activate or deactivate a model/module. Please note that the first three modules MODFLOW, PMPATH and TEXT VIEWER are required and cannot be deactivated. When a module is deactivated, its associated menu item under the Models menu is removed. This feature is useful, when several modules are not used and the Models menu should be kept as short as possible. Deactivating or activating of a module does not affect the model data in any way.
- *Paths* to Simulation Program File: If the user intends to use an executable program located in another position, click the corresponding button and select the desired program from a dialog box.
  Note. The following programs must be located in the same directory as the PEST (PEST-ASP) program: mf2kasp.exe, mf2pest.exe, modbore.exe, par2sen.exe, and pestchek.exe.

2.3.5 Save Plot As

Use *Save Plot As* to save the contents of the worksheet in graphics files. Three graphics formats are available: Drawing Interchange File (DXF), Hewlett-Packard Graphics Language (HP-GL) and Windows Bitmap (BMP). DXF is a fairly standard format developed by Autodesk for exchanging data between CAD systems. HP-GL is a two-letter mnemonic graphics language developed by Hewlett-Packard. Most graphics or word-processing software, and graphics devices can process these graphics formats. To save a plot, use the Format drop-down box to select a graphic format. Then, enter a filename into the File edit field, or click and select a file from a dialog box. When finished, click OK. **Note that in the Map View display mode only the BMP-format may be used.**

2.3.6 Print Plot

This menu item is only activated in the Data Editor. After selecting this item, a Print Plot dialog box is displayed with a preview window. The options are described below.

- Use full page: The plot is scaled to fit the paper; the original aspect ratio will not be changed.
- Center on page: The plot is placed on the center of the page.
- Image Size (millimeters): Specify the width and height of the printed image in millimeters.
- Margins (millimeters): Specify the left and top margins of the image in millimeters.
- Printer: A Printer dialog box allows the user to select an installed printer and specify the print quality, the paper size, source and orientation and other printing parameters.

- Print: Print the contents shown on the preview window.
- Close: Close the Print Plot dialog box without printing.

2.3.7 Animation

This menu item is only activated when the 2D Visualization (*Tools | 2D Visualization*) tool is selected. Before creating an animation sequence, the user should use the Environment Option and Maps Option dialog boxes (refer to Section 2.9 for details) to make sure that the model grid, maps and contours are set properly.

► To create an animation sequence

1. Select *File | Animation* to display an Animation dialog box.
2. In the Animation dialog box, click the open file button to display a Save File dialog box.
   Select an existing frame file or specify a new base file name for the frame files in the dialog box, then click Open. Like a movie, an animation sequence is based on a series of of frames. Each frame is saved by using the filename *basename.nnn*, where *basename* is the base file name and *nnn* is the serial number of the frame files.
   Note. To protect the model data, the frame files must not be saved in the same folder as the model data.
3. Check or clear Create New Frames.
   Check Create New Frames if a new animation sequence should be created. Clear the Create New Frame box if a saved sequence should be played back.
4. Set Delay(s). Delay is the number of seconds between frames.
5. In the Animation dialog box, click OK to start the animation. **PM** will create a frame (image) for each time point at which the simulation results have been saved. When all frames are created, **PM** will repeat the animation indefinitely until the Esc key is pressed.

2.4 The Grid Menu

2.4.1 Mesh Size

Allows the user to generate or modify a model grid using the Grid Editor. See Section 2.1 for how to use the Grid Editor.

2.4.2 Layer Property

The layer properties are defined in the Layer Property dialog box (Fig. 2.14). Many settings of this dialog box depend on the selection between the Block-Centered-Flow (BCF) and Layer Property Flow (LPF) packages. Refer to Section 2.3.4 for details about the BCF and LPF package. When the LPF Package is used, the columns

Transmissivity, Leakance and Storage Coefficient are dimmed to indicate that their settings are ignored, because the LPF package only uses HK, VK, Ss and Sy. When the BCF package is used, the column Vertical Anisotropy is dimmed since it is not supported by the BCF package. The settings of this dialog box are described below.

- Type: The numerical formulations, which are used by the BCF or LPF package to describe groundwater flow, depend on the type of each model layer. The available layer types are:
  - Type 0: The layer is strictly confined. For transient simulations, the confined storage coefficient (specific storage $\times$ layer thickness) is used to calculate the rate of change in storage. Transmissivity of each cell is constant throughout the simulation.
  - Type 1: The layer is strictly unconfined. The option is valid for the first layer only. Specific yield is used to calculate the rate of change in storage for this layer type. During a flow simulation, transmissivity of each cell varies with the saturated thickness of the aquifer.
  - Type 2: A layer of this type is partially convertible between confined and unconfined. Confined storage coefficient (specific storage $\times$ layer thickness) is used to calculate the rate of change in storage, if the layer is fully saturated, otherwise specific yield will be used. Transmissivity of each cell is constant throughout the simulation. Vertical leakage from above is limited if the layer desaturates.
  - Type 3: A layer of this type is fully convertible between confined and unconfined. Confined storage coefficient (specific storage $\times$ layer thickness) is used to calculate the rate of change in storage, if the layer is fully saturated, otherwise specific yield will be used. During a flow simulation, transmissivity of each cell varies with the saturated thickness of the aquifer. Vertical leakage from above is limited if the layer desaturates.

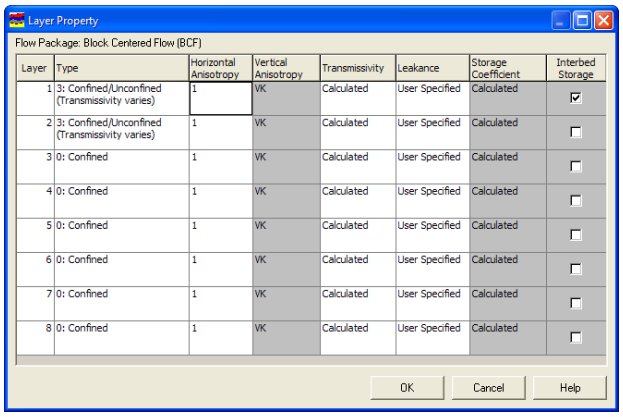

Layer Property
Flow Package: Block Centered Flow (BCF)
Layer
Type
Horizontal Anisotropy
Vertical Anisotropy
Transmissivity
Leakance
Storage Coefficient
Interbed Storage
1 3: Confined/Unconfined (Transmissivity varies) 1 VK Calculated User Specified Calculated
2 3: Confined/Unconfined (Transmissivity varies) 1 VK Calculated User Specified Calculated
3 0: Confined 1 VK Calculated User Specified Calculated
4 0: Confined 1 VK Calculated User Specified Calculated
5 0: Confined 1 VK Calculated User Specified Calculated
6 0: Confined 1 VK Calculated User Specified Calculated
7 0: Confined 1 VK Calculated User Specified Calculated
8 0: Confined 1 VK Calculated User Specified Calculated
OK
Cancel
Help

Fig. 2.14. The Layer Property dialog box

Note that the LPF package uses only two layer types - confined and convertible. Layer type 0 will be interpreted by the LPF package as confined and all other layer types will be interpreted as convertible layers, i.e. the layers are convertible between confined and unconfined.

- Horizontal Anisotropy: The ratio of the horizontal hydraulic conductivity along columns to hydraulic conductivity along rows. The latter is specified by selecting *Parameters* | *Horizontal Hydraulic Conductivity*.
  - When the LPF package is used, a positive Horizontal Anisotropy value indicates that horizontal anisotropy is constant for all cells in the layer and the anisotropy is the specified value. A negative value indicates that horizontal anisotropy can vary at each cell in the layer. The cell-by-cell anisotropy values are specified by selecting *Parameters* | *Horizontal Anisotrop*y.
  - When the BCF package is used, horizontal anisotropy is constant for all cells in the layer and the anisotropy is the absolute value of the specified Horizontal Anisotropy value.
- Vertical Anisotropy: The setting of this column is either VK or VANI.
  - VK indicates that vertical hydraulic conductivity is used for the layer and is to be specified by selecting *Parameters* | *Vertical Hydraulic Conductivity*.
  - VANI indicates that vertical anisotropy is used for the layer and is to be specified by selecting *Parameters* | *Vertical Anisotropy*.
- Transmissivity: MODFLOW (or exactly to say, the BCF package) requires transmissivity (= horizontal hydraulic conductivity $[LT^{-1}] \times$ layer thickness $[L]$) for layers of type 0 or 2. **PM** provides two options for each model layer to facilitate the data input:
  - Set the Transmissivity setting of a layer to *User-Specified*:
    The user-specified transmissivity values of the layer are used in the simulation.
  - Set the Transmissivity setting of a layer to *Calculated*:
    PM calculates transmissivity of the layer by using user-specified horizontal hydraulic conductivity and the elevations of the top and bottom of the layer. The calculated transmissivity values are used in the simulation.
- Leakance: For flow simulations involving more than one model layer, MODFLOW (BCF package) requires the input of the vertical conductance term, known as vertical leakance (VCONT array), between two model layers. MODFLOW uses VCONT to formulate the flow rate equation between two vertically adjacent cells. **PM** provides two options for each model layer to facilitate the data input:
  - Set the Leakance setting of a layer to *User-Specified*:
    The user-specified vertical leakance values are used in the simulation. In the Data Editor, the vertical leakance between the layers i and i+1 is given as the data of the i-th layer. The leakance data are not required for the bottom layer since MODFLOW assumes that the bottom layer is underlain by impermeable material.
  - Set the Leakance setting of a layer to *Calculated*:
    PM calculates vertical leakance by using the rules explained below. The calculated vertical leakance values are used in the simulation.

As illustrated in Fig. 2.15a, when each model layer represents a different hydrostratigraphic unit or when two or more layers represent a single hydrostratigraphic unit, **PM** uses equation 2.1 to calculate the vertical leakance VCONT.

$$VCONT = \frac{2}{\frac{\Delta\nu_k}{(K_z)_{k,i,j}} + \frac{\Delta\nu_{k+1}}{(K_z)_{k+1,i,j}}} \tag{2.1}$$

where $(K_z)_{k,i,j}$ and $(K_z)_{k+1,i,j}$ are the vertical hydraulic conductivity values of layers k and k+1, respectively. The ratio of horizontal to vertical hydraulic conductivity ranging from 1:1 to 1000:1 is common in model application [8]. A summary of hydraulic conductivity values can be found in [109]. It is not uncommon to represent resistance to flow in a low hydraulic conductivity unit (2.15b, semiconfining unit) by lumping the vertical hydraulic conductivity and thickness of the confining unit into a vertical leakance term between two adjacent layers. These kinds of models are often called quasi three-dimensional models, because semi-confining units are not explicitly included in a simulation. In this case the user must manually calculate the VCONT values using equation 2.2 and enter them into the Data Editor.

$$VCONT = \frac{2}{\frac{\Delta\nu_u}{(K_z)_u} + \frac{\Delta\nu_c}{(K_z)_c} + \frac{\Delta\nu_L}{(K_z)_L}} \tag{2.2}$$

where $(K_z)_u$, $(K_z)_c$, and $(K_z)_L$ are the vertical hydraulic conductivity values of the upper layer, semi-confining unit and lower layer, respectively.

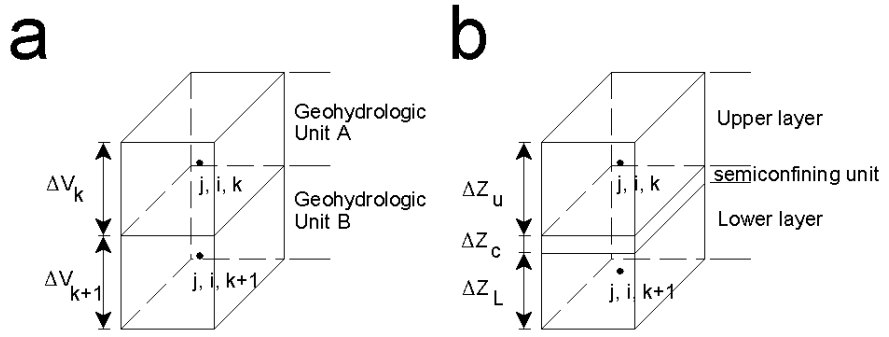


Fig. 2.15. Grid configuration used for the calculation of VCONT

- Storage Coefficient: For transient flow simulations, MODFLOW (BCF package) requires dimensionless storage terms to be specified for each model layer. For a confined layer, these storage terms are given by the confined storage coefficient (=specific storage $[L^{-1}] \times$ layer thickness $[L]$). If the Storage Coefficient setting

is set to Calculated, **PM** uses user-specified specific storage and the elevations of the top and bottom of each layer to calculate the confined storage coefficient. Set the Storage Coefficient flag to User Specified, if you want to specify the confined storage coefficient manually. For an unconfined layer, the storage values are equal to specific yield [−]. The setting of the Storage Coefficient flag has no influence on the specific yield.

- Interbed Storage: **PM** supports the Interbed-Storage package for calculating storage changes from both elastic and inelastic compaction of each model layer. Check the Interbed Storage setting of a specific layer to calculate its storage changes and compaction by using the Interbed-Storage package. Refer to Section 2.6.1.5 for details about this package.

2.4.3 Cell Status

2.4.3.1 IBOUND (MODFLOW)

The flow model MODFLOW requires an IBOUND array, which contains a code for each model cell. A positive value in the IBOUND array defines an active cell (the hydraulic head is computed), a negative value defines a constant head or fixed head cell (the hydraulic head is kept constant at a given value throughout the flow simulation) and the value 0 defines an inactive cell (no flow takes place within the cell). It is suggested to use 1 for active cells, 0 for inactive cells and -1 for constant head cells. Any outer boundary cell, which is not a constant head cell, is automatically a zero flux boundary cell. Flux boundaries with non-zero fluxes are simulated by assigning appropriate infiltration or pumping wells in the corresponding cell via the well package.

For constant head cells, the initial hydraulic head remains the same throughout the simulation. The initial hydraulic head is specified by selecting *Parameters | Initial and Prescribed Hydraulic Heads*. A constant head boundary exists whenever an aquifer is in direct hydraulic contact with a river, a lake, or a reservoir in which the water (groundwater) level is known to be constant. It is important to be aware that a constant head boundary can provide inexhaustible supply or sink of water. A groundwater system may get or lose as much water as necessary from or to such a boundary without causing any change of hydraulic heads in the constant head boundary. In some situations, this may be unrealistic. Therefore care must be taken when using constant head boundaries and it is suggested to avoid using this boundary condition on the upstream side of the groundwater flow direction. Consider using the General-Head Boundary or the Time-Variant Specified-Head packages, if the hydraulic head at the constant head boundary varies with time. Head-dependent boundary conditions are modeled by means of the general head boundary, river, or drain package.

If it is planned to use MOC3D, the user should be aware that MOC3D allows one to specify zones along constant head boundaries, which are associated with different source concentrations. Zones are defined within the IBOUND array by specifying unique negative values. For example, if a model has three zones, one will use -1, -2 and -3 for the constant head cells. Note that the associated concentrations must be

specified by selecting *Models* | *MOC3D* | *Sink/Source Concentration* | *Fixed-Head Cells.*

2.4.3.2 ICBUND (MT3D/MT3DMS)

The transport models MT3D, MT3DMS, and RT3D require an ICBUND array, which contains a code for each model cell. A positive value in the ICBUND array defines an active concentration cell (the concentration varies with time and is calculated), a negative value defines a constant-concentration cell (the concentration is constant) and the value 0 defines an inactive concentration cell (no transport simulation takes place at such cells). It is suggested to use the value 1 for an active concentration cell, -1 for a constant-concentration cell, and 0 for an inactive concentration cell. Note that the ICBUND array applies to all species if MT3DMS or RT3D is used. Other types of boundary conditions are implemented by assigning concentrations to inflows (see sections 2.6.6.6 and 2.6.2.8) or assigning a mass-loading rate to a cell (Section 2.6.2.9).

MT3D, MT3DMS, and RT3D automatically convert no-flow or dry cells to inactive concentration cells. Active variable-head cells can be treated as inactive concentration cells to minimize the area needed for transport simulation, as long as the solute transport is insignificant near those cells. For constant-concentration cells, the initial concentration remains the same at the cell throughout the simulation. A constant head cell may or may not be a constant-concentration cell. The initial concentration is specified by selecting *Models* | *MT3D* | *Initial Concentration*, *Models* | *MT3DMS* | *Initial Concentration*, or *Models* | *RT3D* | *Initial Concentration.*

2.4.4 Top of Layers (TOP)

The top elevation of a layer is required when one of the following conditions applies. **PM** will check these conditions (except the last one) prior to running a model simulation.

1. The BCF package is selected and layer type 2 or 3 is used.
2. The BCF package is selected and VCONT to the underlying layer is calculated by **PM**.
3. The BCF package is selected and T or S is calculated by **PM**.
4. The LPF package is used.
5. One of the programs – PMPATH, MT3D, MT3DMS, MOC3D, RT3D, PHT3D or 3D Master (for 3D-Visualization) – will be used.

2.4.5 Bottom of Layers (BOT)

The bottom elevation of a layer is required when one of the following conditions applies. **PM** will check these conditions (except the last one) prior to running a model simulation.

1. The BCF package is selected and layer type 2 or 3 is used.

2. The BCF package is selected and VCONT to the underlying layer is calculated by **PM**.
3. The BCF package is selected and T or S is calculated by **PM**.
4. The LPF package is used.
5. One of the programs – PMPATH, MT3D, MT3DMS, MOC3D, RT3D, PHT3D or 3D Master (for 3D-Visualization) – will be used.

2.5 The Parameters Menu

This menu is used to input time, initial hydraulic head values, and aquifer parameters such as HK or VK. Depends on the settings of the layer properties (Section 2.4.2), it is possible that an aquifer parameter is required only for certain model layers or is not required for any of the model layers. In the latter case, the corresponding menu item will be dimmed. In the former case, the Data Editor will display a short indicative message *"data of this layer will be used in the simulation"* or *"data of this layer will NOT be used in the simulation."* on the status bar to indicate whether an aquifer parameter is required for the layer being edited.

2.5.1 Time

Selecting this menu item to display a Time Parameters dialog box. The appearance of this dialog box is affected by the setting of the Modflow version (Section 2.3.4).

When the Modflow Version is set to "MODFLOW-2000/MODFLOW-2005", the *Transient* column appears in the table of this dialog box and the Simulation Flow Type group of this dialog box is dimmed and deactivated (Fig. 2.16) since MODFLOW-2000 allows individual stress periods in a single simulation to be either transient or steady state instead of requiring the entire simulation to be either steady state or transient. Steady state and transient stress periods can occur in any order. Commonly the first stress period is steady state and produces a solution that is used as the initial condition for subsequent transient stress periods.

When the Modflow Version is not set to "MODFLOW-2000/MODFLOW-2005", the *Transient* column disappears and all stress periods are either steady-state or transient, which is controlled by the options of the Simulation Flow Type group (Fig. 2.17). The columns of this dialog box are described below.

- *Period, Active, Length, Time Step*: MODFLOW divides the simulation time into stress periods, which are, in turn, divided into time steps. Check the Active box to activate a stress period. For each stress period, the user has the option of changing parameters associated with head-dependent boundary conditions in the River, Stream, Drain, Evapotranspiration, General-Head Boundary, and Time-Variant Specified-Head Boundary packages, as well as the recharge rates in the Recharge package and pumping rates in the Well package. For transport simulations, the user may change mass-loading rates (MT3DMS only) and source concentrations associated with the fluid sources and sinks.

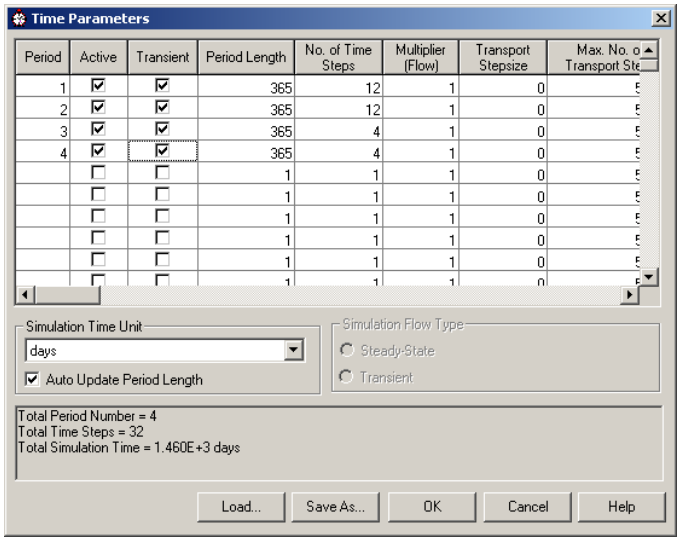


Fig. 2.16. The Time Parameters dialog box for MODFLOW-2000/MODFLOW-2005

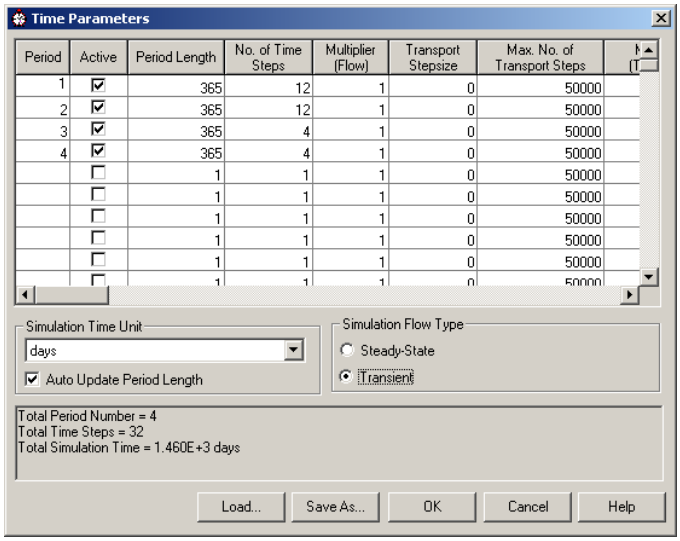


Fig. 2.17. The Time Parameters dialog box for MODFLOW-96

The length of stress periods and time steps is not relevant to steady state flow simulations. However, if transport simulations need to be done at a later time, the actual period length should be entered.

- *Transient*: Check the Transient box, if a stress period is transient. Clear the Transient box, if a stress period is steady-state.

- *Multiplier (Flow)*: MODFLOW allows the time step to increase as the simulation progresses. It uses the following equations to increase the lengths of time steps as a geometric progression.

$$\Delta t_1 = PERLEN \cdot \frac{TSMULT - 1}{TSMULT^{NSTP} - 1} \tag{2.3}$$

$$\Delta t_{m+1} = TSMULT \cdot \Delta t_m \tag{2.4}$$

  where $PERLEN$ is the length of a stress period, $TSMULT$ is the time step multiplier, $NSTP$ is the number of time steps, and Δt_m is the length of the m-th time step within a stress period.
- *Transport Step size*: The transport models further divide each time step into smaller time increments, called transport steps. Because the explicit numerical solution of the solute-transport equation has certain stability criteria associated with it, the length of a time step used for a flow solution may be too large for a transport solution. Each time step must, therefore, be divided into smaller transport steps. For explicit solutions (e.g., when the Generalized Conjugate Gradient solver is not used in MT3DMS), the transport step sizes in the table are used for the simulation. Considering stability criteria, the transport models always calculate a maximum allowed transport step size $Deltat_{max}$. Usually the smallest cell containing sinks will be the one, which determines $Deltat_{max}$. Therefore in transport simulations variable cell sizes are not always beneficial. Setting the transport step size in the table to zero or to a value greater than $Deltat_{max}$ will cause $Deltat_{max}$ to be used for the simulation. For details about the stability criteria associated with the explicit transport-solution, refer to [74], [117], or [118]. For implicit solutions in MT3DMS (i.e. when the Generalized Conjugate Gradient solver is used), the transport step sizes in the table are the initial transport step size in each flow time step. The subsequent transport step size may increase or remain constant depending on the user-specified transport step size multiplier (see below). If the transport step size is specified as zero, the model-calculated value, based on the user-specified Courant number in the Advection Package (MT3DMS) dialog box, is used.
- *Max. No. of Transport Steps*: If the number of transport steps within a flow time step exceeds the maximum number, the simulation is terminated.
- *Multiplier (Transport)* is the multiplier for successive transport steps within a flow time step. This value is used by MT3DMS for the case that the Generalized Conjugate Gradient solver and the solution option for the advection term is the finite-difference method (see Section 2.6.2.3).
- *Simulation Time Unit*: Each time when the time unit in the Simulation Time Unit group is changed, **PM** will update the period length in the table, if *Auto Update Period Length* is checked. Note that changing the time unit does not affect the user-specified parameter values.
- *Simulation Flow Type*: **PM** allows to perform steady state or transient flow simulations by selecting an option from the Simulation Flow Type group. It is possible to run a steady state simulation over several stress periods. In this case, a steady state solution is calculated for each stress period.

- *Save As and Load*: Using these buttons, the user can save or load the contents of the table in or from a time parameter file or a ASCII time parameter file. The format of the ASCII time parameter file is given in Section 6.2.5.

2.5.2 Initial & Prescribed Hydraulic Heads

MODFLOW requires initial hydraulic heads at the beginning of a flow simulation. Initial hydraulic heads at constant head cells are used as specified head values of those cells and remain constant throughout the flow simulation.

For transient flow simulations, the initial heads must be the actual values, since they are used to account for the storage terms. For steady-state flow simulations, the initial heads are used as starting values for the iterative equation solvers. The initial heads at the constant head cells must be the actual values while all other values can be set at an arbitrary level. For an unconfined or convertible layer (layer type 1 or 3), the initial hydraulic head of a constant head cell should be higher than the elevation of the cell bottom, because MODFLOW does not convert a dry fixed-head cell to an inactive cell. If any constant-head cell becomes dry, MODFLOW will stop the flow simulation and write a message ”CONSTANT-HEAD CELL WENT DRY - SIMULATION ABORTED” into the run listing file OUTPUT.DAT.

2.5.3 Horizontal Hydraulic Conductivity and Transmissivity

Horizontal hydraulic conductivity is required for layers of types 1 or 3. Transmissivity is required for layers of types 0 or 2. Horizontal hydraulic conductivity is the hydraulic conductivity along model rows. It is multiplied by an anisotropy factor specified in the Layer Property dialog box (Section 2.4.2) to obtain the hydraulic conductivity along model columns. Typical values and ranges of horizontal hydraulic conductivity for different types of soils are given in many groundwater textbooks, for example Freeze and Cherry [46], Spitz and Moreno [109] and Fetter [44].

For layers of types 0 or 2, **PM** uses the horizontal hydraulic conductivity and layer thickness to calculate transmissivity if the corresponding Transmissivity setting in the Layer Property dialog box (Section 2.4.2) is set to *Calculated*. The user-specified transmissivity values of a model layer are used in the simulation if the Transmissivity setting of that layer is set to *User-specified*.

2.5.4 Horizontal Anisotropy

The Layer-Property Flow (LPF) package supports the use of the cell-by-cell horizontal anisotropy, which is the ratio of horizontal hydraulic conductivity along columns to hydraulic conductivity along rows. The latter is specified by selecting *Parameters | Horizontal Hydraulic Conductivity*. The menu item Horizontal Anisotropy is dimmed and cannot be used with the Block-Centered Flow (BCF) package.

The cell-by-cell horizontal anisotropy values of a layer are used, only when the Horizontal Anisotropy value of the layer in the Layer Options dialog box (Fig. 2.14; page 28) is negative.

2.5.5 Vertical Leakance and Vertical Hydraulic Conductivity

The BCF package uses the vertical leakance (VCONT) values to formulate the flow rate equation between two vertically adjacent cells. As discussed in Section 2.4.2, the user may either specify the vertical leakance values directly or specify the vertical hydraulic conductivity values and let **PM** calculate the required VCONT values.

When *Vertical Leakance* of a layer in the Layer Property dialog box (Fig. 2.14) is User-specified, the user-specified vertical leakance values of that layer are used in the simulation. When *Vertical Leakance* is calculated, **PM** calculates the VCONT values and uses them in the simulation. Refer to Section 2.4.2 for details.

2.5.6 Vertical Anisotropy and Vertical Hydraulic Conductivity

The Layer-Property Flow (LPF) package supports the use of the cell-by-cell vertical hydraulic conductivity or vertical anisotropy, which is the ratio of horizontal hydraulic conductivity along rows to vertical hydraulic conductivity for the model layer. The menu item Vertical Anisotropy is dimmed and cannot be used with the Block-Centered Flow (BCF) package.

When Vertical Anisotropy of a layer in the Layer Property dialog box (Fig. 2.14) is VK, the cell-by-cell vertical hydraulic conductivity of that layer is used in the simulation. When Vertical Anisotropy is VANI, the cell-by-cell vertical anisotropy of the layer is used.

2.5.7 Effective Porosity

If the total unit volume V of a soil matrix is divided into the volume of the solid portion V_s and the volume of voids V_v, the porosity n is defined as $n = V_v/V$. Effective porosity (with the respect to flow through the medium) is normally smaller than porosity, because part of the fluid in the pore space is immobile or partially immobile. This may occur when the flow takes place in a fine-textured medium where adhesion (i.e., the attraction to the solid surface of the porous matrix by the fluid molecules adjacent to it) is important. On a more macroscopic scale the effective porosity also has to accommodate the fact that unresolved conductivity variations lead to a reduction of effective porosity.

Transport models, for example PMPATH or MT3DMS, use effective porosity to calculate the average velocity of the flow through the porous medium. If a dual-porosity system is simulated by MT3DMS, effective porosity should be specified as the portion of total porosity filled with mobile water and the ”immobile” porosity is defined through *Models* | *MT3DMS* | *Chemical Reaction*. A summary of representative porosity values for different soil types can be found in Zheng and Bennett [118] or Domenico and Schwartz [41].

2.5.8 Specific Storage, Storage Coefficient and Specific Yield

For transient flow simulations, MODFLOW requires dimensionless storage terms specified for each layer of the model. For a steady state simulation, these menu items are not used and are therefore dimmed.

In a confined layer, the storage term is given by storativity or confined storage coefficient (= specific storage $[L^{-1}] \times$ layer thickness $[L]$). The storativity is a function of the compressibility of the water and the elastic property of the soil matrix. The specific storage or specific storativity is defined as the volume fraction of water that a unit column of aquifer releases from storage under a unit decline in hydraulic head. The specific storage ranges in value from 3.3×10^{-6} $[m^{-1}]$ of rock to 2.0×10^{-2} $[m^{-1}]$ of plastic clay (Domenico [40]).

Layers of types 0, 2 and 3 require the confined storage coefficient. **PM** uses specific storage and the layer thickness to calculate the confined storage coefficient, if the corresponding Storage Coefficient setting in the Layer Property dialog is *Calculated*. By setting the *Storage Coefficient* setting to *User Specified* and selecting *Parameters* | *Storage Coefficient*, you can specify the confined storage coefficient directly.

In a phreatic aquifer (Layers of types 2 and 3), the storage term is given by specific yield or drainable porosity. Specific yield is defined as the volume of water that an unconfined aquifer releases from storage per unit surface area of aquifer per unit decline in the water table. Specific yield is a function of porosity (and is not necessarily equal to porosity), because a certain amount of water is held in the soil matrix and cannot be removed by gravity drainage. Refer to Spitz and Moreno [109] for a summary of values of specific yield. Refer to Bear [12][13] or Freeze and Cherry [46] for detailed explanation of storage terms and their definitions.

2.5.9 Bulk Density

2.5.9.1 Layer by Layer

The layer-by-layer bulk-density data are used by the Chemical Reaction package of MT3D or RT3D (version 1) for calculating the retardation factor or for calculating the first-order irreversible (radioactive decay or biodegradation) rate of the adsorbed phase. Refer to Section 2.6.6.4 for details.

2.5.9.2 Cell by Cell

The cell-by-cell bulk-density data are used by the Chemical Reaction package of MT3DMS, MT3D99, PHT3D, SEAWAT, and RT3D (version 2 and later) for simulating sorption effects.

2.6 The Models Menu

2.6.1 MODFLOW

2.6.1.1 MODFLOW | Flow Packages | Drain

The Drain package is used to simulate effects of features such as agricultural drains, which remove groundwater from aquifer at a rate proportional to the head difference between the aquifer and the drain. When the hydraulic head in the aquifer is greater than the drain elevation, ground water flows into the drain and is removed from the groundwater model. Discharge to the drain is zero when the hydraulic head is lower than or equal to the median drain elevation. Recharge from the drain is always zero, regardless of the hydraulic head in the aquifer.

Using the Data Editor, a drain system is defined by using the Cell-by-Cell or Polygon input methods to assign parameters to model cells or by using the Polyline input method and assigning parameters to vertices of the polylines along the trace of drain system. The input parameters are assumed to be constant during a given stress period. For transient flow simulations involving several stress periods, the input parameters can be different from period to period. The input methods require different parameters as described below.

- When using the Polyline input method, right-click on a vertex to specify its properties in the Drain Parameters dialog box (Fig. 2.18). If the properties are assigned to one vertex only, the properties of all vertices of the polyline are assumed to be the same. The settings of the dialog box are described below.
  - *Layer Option and Layer Number*: Layer Option controls how the layer number of a drain is determined.
    * If Layer Option is ”Assign layer number manually”, the value of *Layer Number* defines the model layer number for all model cells downstream from a vertex until the next vertex redefines the layer number.

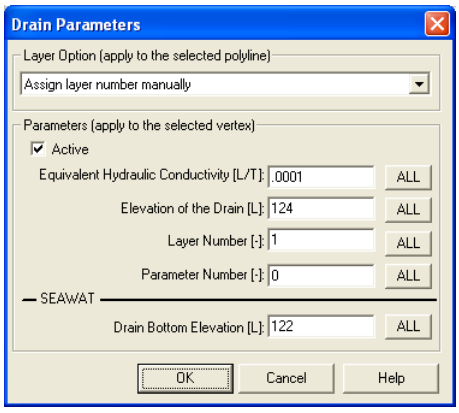


Fig. 2.18. The Drain Parameters dialog box

  * If Layer Option is "Assign layer number automatically", the drain is assigned to a layer where the drain elevation d (see below) is located between the top and bottom of the layer. The layer number is set to 1 if d is higher than the top of the first layer. The layer number is set to the last layer if d is lower than the bottom of the last layer.
- *Active*: Check this box to activate a vertex. Clear the Active box to deactivate a vertex. The properties of an active vertex will be used in the simulation. The properties of an inactive vertex are ignored.
- *Equivalent Hydraulic Conductivity (K) [LT^{-1}]* and *Elevation of the Drain (d) [L]*: The value K describes all of the head loss between the drain and the aquifer. It depends on the material and characteristics of the drain itself and the immediate environment. Since the Drain package requires the input of drain hydraulic conductance (C_d) and drain elevation (d) to each cell of a drain, the input values K and d at active vertices are linearly interpolated or extrapolated to each cell along the trace of the polyline and the value C_d is obtained by

$$C_d = K \cdot L \tag{2.5}$$

  where L is the length of the drain within a cell. The discharge rate to a drain cell (Q_d) is calculated by

$$Q_d = C_d \cdot (h - d) \tag{2.6}$$

  where h is the hydraulic head in a drain cell. By default, MODFLOW saves the calculated discharge rates in the BUDGET.DAT.
- *Parameter Number [$-$]*: Since C_d is usually unknown, it must be estimated. Parameter Number is used to group cells, where the C_d values are to be estimated by the parameter estimation programs MODFLOW-2000 (Section 2.6.7) or PEST (Section 2.6.8). Refer to the corresponding sections for parameter estimation steps. The value of Parameter Number is assigned to all model cells downstream from a vertex until the next vertex redefines the parameter number.
- *Drain Bottom Elevation [L]*: This value is used by SEAWAT to calculate reference head considering the density effect to to accurately simulate the flow of variable-density ground water to a drain.
- The *ALL* button: Click the ALL button of a property to copy the property value to all other active vertices.

- When using the Cell-by-cell or Polygon input methods, the following values are to be assigned to model cells of a drain system. See the explanations above for the definition of the input values.
  - *Drain hydraulic conductance (C_d) [L^2T^{-1}]*,
  - *Elevation of the Drain (d) [L]*,
  - *Parameter Number [$-$]*, and
  - *Drain Bottom Elevation [L]*.

2.6.1.2 MODFLOW | Flow Packages | Evapotranspiration

The Evapotranspiration package simulates the effects of plant transpiration and direct evaporation in removing water from the saturated groundwater regime.

Evapotranspiration is defined by assigning the following parameters to each vertical column of cells. The input parameters are assumed to be constant during a given stress period. For transient flow simulations involving several stress periods, the input parameters can be different from period to period. Note that the user may move to other layers within the Data Editor and examine the grid configuration in each layer, although the values are specified for each vertical column of cells.

- Maximum ET Rate (R_{ETM}) [LT^{-1}],
- Elevation of the ET Surface (hs) [L],
- ET Extinction Depth (d) [L],
- Layer Indicator (I_{ET}) [$-$], and
- Parameter Number [$-$].

Parameter Number is used to group cells, where the R_{ETM} values are to be estimated by the parameter estimation programs PEST (Section 2.6.8) or MODFLOW-2000 (Section 2.6.7). Refer to the corresponding sections for parameter estimation steps.

The Evapotranspiration package removes water from the saturated groundwater regime based on the following assumptions:

1. When groundwater table is at or above the elevation of the ET surface hs, evapotranspiration loss from the groundwater table is at the maximum ET Rate R_{ETM};
2. No evapotranspiration occurs when the depth of the groundwater table below the elevation of the ET surface exceeds the ET extinction depth d; and
3. In between these two extremes evapotranspiration varies linearly with the groundwater table elevation.

These assumptions can be expressed in the equation form:

$$\begin{aligned} R_{ET} &= R_{ETM} && \text{if} \quad h > h_s \\ R_{ET} &= 0 && \text{if} \quad h < h_s - d \\ R_{ET} &= R_{ETM} \cdot \left[\frac{h - (h_s - d)}{d} \right] && \text{if} \quad h_s - d \leq h \leq h_s \end{aligned} \tag{2.7}$$

where R_{ET} [LT^{-1}] is the evapotranspiration rate per unit surface area of groundwater table. The evapotranspiration flow rate (Q_{ET} [L^3T^{-1}]) drawn from a model cell is

$$Q_{ET} = R_{ET} \cdot DELR \cdot DELC \tag{2.8}$$

where $DELR \cdot DELC$ is the map area of a model cell. Q_{ET} is drawn from only one cell in the vertical column beneath the map area. The Evapotranspiration package provides two options for specifying the cell in each vertical column of cells where evapotranspiration is drawn from:

1. Evapotranspiration is always drawn from the top layer of the model.
2. Vertical distribution of evapotranspiration is specified in the Layer Indicator Array. I_{ET} defines the layer where evapotranspiration is drawn from. the groundwater table elevation.

In either case the Q_{ET} has no influence on the simulation if the designated cell is either a no-flow (inactive) cell or a constant head cell. You can select an option in the Evapotranspiration Package dialog box. The layer indicator array is needed only when the second option is used.

2.6.1.3 MODFLOW | Flow Packages | General-Head Boundary

The General-Head Boundary (GHB) package is used to simulate head-dependent flow boundaries (Cauchy boundary conditions), where flow into or out of a GHB-cell from an external source is provided in proportion to the difference between the head in the cell and the head assigned to the external source.

Using the Data Editor, a general-head boundary is defined by using the Cell-by-Cell or Polygon input methods to assign parameters to model cells or by using the Polyline input method and assigning parameters to vertices of the polylines along the trace of the boundary. The input parameters are assumed to be constant during a given stress period. For transient flow simulations involving several stress periods, the input parameters can be different from period to period. The input methods require different parameters as described below.

- When using the Polyline input method, right-click on a vertex to specify its properties in the General Head Boundary Parameters dialog box (Fig. 2.19). If the properties are assigned to one vertex only, the properties of all vertices of the polyline are assumed to be the same. The settings of the dialog box are described below.
  - *Layer Option* and *Layer Number*: Layer Option controls how the layer number of a general head boundary is determined.

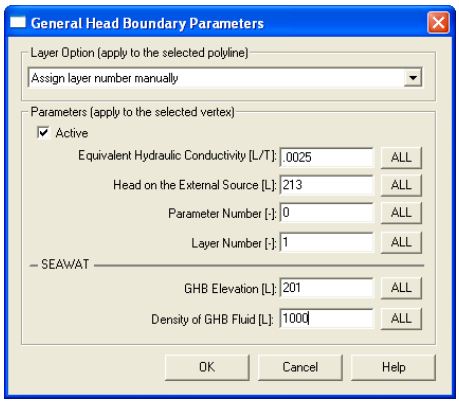


Fig. 2.19. The General Head Boundary Parameters dialog box

  * If Layer Option is "Assign layer number manually", the value of *Layer Number* defines the model layer number for all model cells downstream from a vertex until the next vertex redefines the layer number.
  * If Layer Option is "Assign layer number automatically", the boundary is assigned to a layer where Head on Boundary h_b (see below) is located between the top and bottom of the layer. The layer number is set to 1 if h_b is higher than the top of the first layer. The layer number is set to the last layer if h_b is lower than the bottom of the last layer.

– *Active*: Check this box to activate a vertex. Clear the Active box to deactivate a vertex. The properties of an active vertex will be used in the simulation. The properties of an inactive vertex are ignored.
– *Equivalent Hydraulic Conductivity (K) [LT^{-1}]* and *Head on the External Source (h_b) [L]*: The value K depends on the material and characteristics of the medium between the external source and the model. Since the GHB package requires the input of GHB hydraulic conductance (C_b) and head on the external source (h_b) to each cell of a general-head boundary, the input values K and h_b at active vertices are linearly interpolated or extrapolated to each cell along the trace of the polyline and the value C_b is obtained by

$$C_b = K \cdot L \tag{2.9}$$

where L is the length of the general-head boundary within a cell. Flow through a GHB-cell Q_b [L^3T^{-1}] is calculated by

$$Q_b = C_d \cdot (h_b - h) \tag{2.10}$$

where h is the hydraulic head in the aquifer. By default, MODFLOW saves the calculated flow rates in the BUDGET.DAT. Since the GHB package does not limit the value of flow in either direction, a GHB-cell is equivalent to a constant head cell if a very large C_b is used. Therefore care must be used in utilizing the GHB package to insure that unrealistic flows into or out of the groundwater system do not develop during the course of simulation.
– *Parameter Number [$-$]*: Since C_b is usually unknown, it must be estimated. Parameter Number is used to group cells, where the C_b values are to be estimated by the parameter estimation programs PEST (Section 2.6.8) or MODFLOW-2000 (Section 2.6.7). Refer to the corresponding sections for parameter estimation steps. The value of Parameter Number is assigned to all model cells downstream from a vertex until the next vertex redefines the parameter number.
– *GHB Elevation [L]*: This the elevation of the general-head boundary from which the equivalent reference head is calculated. This value is required by SEAWAT to accurately calculate the flow of variable-density groundwater to the general-head boundary.
– *Density of GHB Fluid [M/L^3]*: This value represents the prescribed density of fluid entering the groundwater system from the general-head boundary. This value is used by SEAWAT only if it is running in a *uncoupled*

mode, i.e., the density-effect of all species are turned off (see 2.6.2.1) and the *Density of general-head boundary fluid* options in the Simulation Settings (MT3TMS/SEAWAT) dialog box (see Fig. 2.46 on p. 89) is set as *User-Specified in the GHB Package*.
  - The ALL button: Click the ALL button of a property to copy the property value to all other active vertices.
- When using the Cell-by-cell or Polygon input methods, the following values are to be assigned to model cells of a general-head boundary. See the explanations above for the definition of the input values.
  - *GHB hydraulic conductance* C_b $[L^2T^{-1}]$,
  - *Head on the External Source* h_b $[L]$,
  - *Parameter Number* $[-]$,
  - *GHB Elevation* $[L]$, and
  - *Density of GHB Fluid* $[M/L^3]$

2.6.1.4 MODFLOW | Flow Packages | Horizontal-Flow Barrier

The Horizontal-Flow Barrier package simulates thin low-permeability geologic features, such as vertical faults or slurry walls, which impede the horizontal flow of groundwater. These geologic features are approximated as a series of horizontal-flow barriers conceptually situated on the boundaries between pairs of adjacent cells in the finite-difference grid. Refer to Hsieh and Freckleton [66] for the numerical implementation of the Horizontal-Flow Barrier package.

A horizontal-flow barrier is defined by assigning the following values to a model cell in the Horizontal-Flow Barrier Package dialog box (Fig. 2.20). The location and the parameters of the barrier are assumed to be constant for the entire simulation.

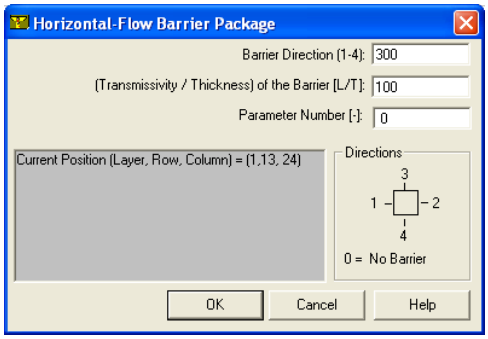


Fig. 2.20. The Horizontal-Flow Barrier dialog box

- Barrier Direction [-]: The barrier direction indicates the cell face where the barrier is located. To erase an existing barrier, use zero for the barrier direction.

- (Hydraulic Conductivity/Thickness) of the barrier TDW $[T^{-1}]$ or (Transmissivity / Thickness) of the barrier TDW $[LT^{-1}]$: The TDW represents the hydraulic characteristic of the barrier. If a layer is unconfined (type 1 or 3) or if MODFLOW-2000 is used, TDW is the barrier hydraulic conductivity divided by the thickness of the barrier. If a layer is confined (type 0 or 2), TDW is the barrier transmissivity divided by the thickness of the barrier.
- *Parameter Number [−]*: Parameter Number is used to group cells, where the TDW values are to be estimated by the parameter estimation programs PEST (Section 2.6.8) or MODFLOW-2000 (Section 2.6.7). Refer to the corresponding sections for parameter estimation steps.

2.6.1.5 MODFLOW | Flow Packages | Interbed Storage

For steady state flow simulations, this menu item is not used and is therefore dimmed.

Groundwater is released from storage under conditions of decreasing hydraulic head. The released water volume is proportional to the compressibility of the soil matrix and water, because a reduction of the hydraulic head results in an increase in the effective stress on the soil skeleton and a decrease of the water pressure. Increasing effective stress on the soil skeleton results in deformation (compaction) of the soil matrix. The Interbed Storage (IBS) package [78] calculates the water volume released from storage and simulates elastic and inelastic compaction of compressible fine-grained beds in an aquifer due to groundwater extraction. The term ”interbed” is used to denote a poorly permeable bed within a relatively permeable aquifer (Fig. 2.21). The interbeds are assumed to consist primarily of highly compressible clay and silt beds from which water flows vertically to adjacent coarse-grained beds.

To incorporate the calculation of interbed storage of a layer, check the Interbed Storage flag in the Layer Property dialog box (see Section 2.4.2). Using the Cell-

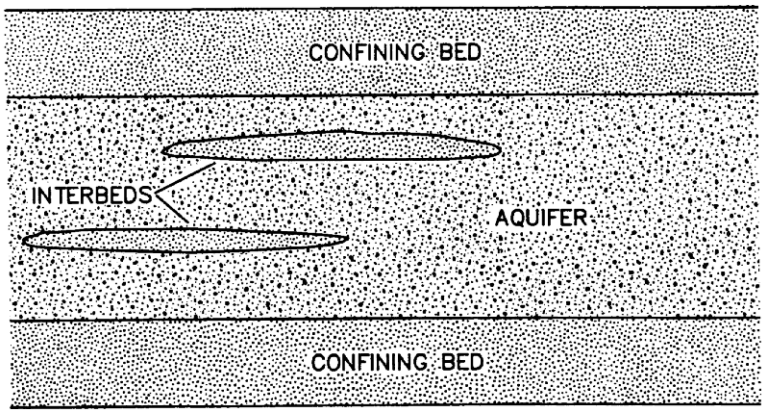


Fig. 2.21. Types of fine-grained beds in or adjacent to aquifers. Beds may be discontinuous interbeds or continuous confining beds. Adapted from Leake and Prudic [78].

by-cell or Polygon input methods of the Data Editor, the following properties of interbeds are specified to model cells.

- Preconsolidation Head or preconsolidation stress H_c $[L]$: Preconsolidation head is the previous minimum head value in the aquifer. For any model cells in which the specified preconsolidation head is greater than the initial hydraulic head, the value of the preconsolidation head will be set to that of the initial hydraulic head; When compressible fine-grained sediments are stressed beyond a previous maximum stress (preconsolidation stress), compaction is permanent (inelastic).
- Elastic Storage Factor S_{fe} $[-]$:
  - For a confined aquifer, the elastic compaction or expansion of sediments is proportional or nearly proportional to changes in hydraulic head values in the aquifer. The IBS package uses the following equation to calculate the change in the thickness Δb $[L]$ of the interbed (positive for compaction and negative for expansion):

$$\Delta b = -\Delta h \cdot S_{fe} = -\Delta h \cdot S_{ske} \cdot b_0 \tag{2.11}$$

    where Δh $[L]$ is change in hydraulic head, positive for increase; S_{ske} $[L^{-1}]$ is the skeletal component of elastic specific storage; b_0 is the thickness of the interbed.
  - For an unconfined aquifer, the elastic compaction or expansion of sediments can be expressed as

$$\Delta b = -\Delta h \cdot S_{fe} = -\Delta h \cdot (1 - n + n_w) \cdot S_{ske} \cdot b_0 \tag{2.12}$$

    where n $[-]$ is porosity and n_w $[-]$ is moisture content above water table as a fraction of total volume of porous medium.
- Inelastic Storage Factor S_{fv} $[-]$:
  - For a confined aquifer, the IBS package uses the following equation in analogy to equation 2.11 to calculate the approximate inelastic compaction $\Delta b*$ $[L]$:

$$\Delta b^* = -\Delta h \cdot S_{fv} = -\Delta h \cdot S_{skv} \cdot b_0 \tag{2.13}$$

    where S_{skv} $[L^{-1}]$ is the skeletal component of inelastic specific storage.
  - For an unconfined aquifer, the inelastic compaction of sediments can be expressed as

$$\Delta b* = -\Delta h \cdot S_{fv} = -\Delta h \cdot (1 - n + n_w) \cdot S_{skv} \cdot b_0 \tag{2.14}$$

    where n $[-]$ is porosity and n_w $[-]$ is moisture content above water table as a fraction of total volume of porous medium.
- Starting Compaction $[L]$: Compaction values computed by the IBS package are added to the starting compaction so that stored values of compaction and land subsidence may include previous components. The starting compaction does not affect the calculation of storage changes or resulting compaction.

- Parameter Number $[-]$: Parameter Number is used to group cells, where the s_{fv} values are to be estimated by the parameter estimation programs PEST (Section 2.6.8) or MODFLOW-2000 (Section 2.6.7). Refer to the corresponding sections for parameter estimation steps.

2.6.1.6 MODFLOW | Flow Packages | Recharge

The Recharge package is designed to simulate distributed recharge to the groundwater system. Recharge is defined by assigning the following data to each vertical column of cells. The input parameters are assumed to be constant during a given stress period. For transient flow simulations involving several stress periods, the input parameters can be different from period to period. Note that the user may move to other layers within the Data Editor and examine the grid configuration in each layer, although the values are specified for each vertical column of cells.

- Recharge Flux I_R $[LT^{-1}]$
- Layer Indicator I_{RCH} $[-]$
- Parameter Number $[-]$ Parameter Number is used to group cells, where the I_R values are to be estimated by the parameter estimation programs PEST (Section 2.6.8) or MODFLOW-2000 (Section 2.6.7). Refer to the corresponding sections for parameter estimation steps.

MODFLOW uses I_R to calculate the recharge flow rate (Q_R $[L^3T^{-1}]$) applied to the model cell:

$$Q_R = I_R \cdot DELR \cdot DELC \tag{2.15}$$

where $DELR \cdot DELC$ is the map area of a model cell. In MODFLOW, the recharge rate Q_R is applied to a single cell within a vertical column of cells. In the simplest situation, the water table is located in the top layer of the model, the top layer is designated as unconfined and an array of Recharge Flux I_R is specified for that layer. Problems may arise, when the water table cuts across layers. To solve this kind of problems, the Recharge package provides three options for specifying the cell in each vertical column of cells that receives the recharge. The user can select an option from the Recharge Package dialog box (Fig. 2.22):

1. Recharge is only applied to the top grid layer.
2. Vertical distribution of recharge is specified in the Layer Indicator array I_{RCH}, which defines the layer where recharge is applied.
3. Recharge is applied to the highest active cell in each vertical column. The user does not have to predetermine the layer to which recharge should be applied. The appropriate layer is automatically selected by the Recharge package. If the highest active cell is a constant-head cell recharge will be intercepted and cannot go deeper.

Refer to the description of the Recharge package in McDonald and Harbaugh [85] for an example of using these options.

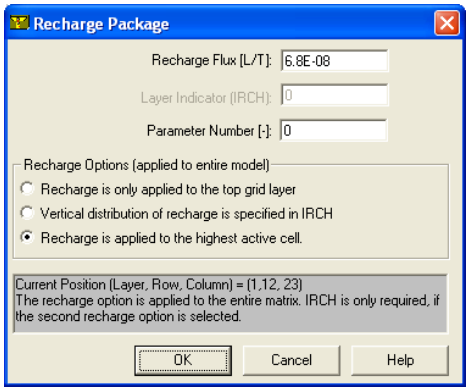

Recharge Package
Recharge Flux [L/T]:
6.8E-08
Layer Indicator (IRCH):
0
Parameter Number [-]:
0
Recharge Options (applied to entire model)
Recharge is only applied to the top grid layer
Vertical distribution of recharge is specified in IRCH
Recharge is applied to the highest active cell.
Current Position (Layer, Row, Column) = (1,12, 23)
The recharge option is applied to the entire matrix. IRCH is only required, if the second recharge option is selected.
OK
Cancel
Help

Fig. 2.22. The Recharge Package dialog box

2.6.1.7 MODFLOW | Flow Packages | Reservoir

The Reservoir package [43] is designed for cases where reservoirs are much greater in area than the area represented by individual model cells. More than one reservoir can be simulated using this package. The area subject to inundation by each reservoir is specified by assigning the reservoir number to selected cells. For reservoirs that include two or more areas of lower elevation separated by areas of higher elevation, the filling of part of the reservoir may occur before spill-ing over to an adjacent area. The package can simulate this process by specifying two or more reservoirs in the area of a single reservoir.

Using the Data Editor, reservoirs are defined by using the Cell-by-Cell or Polygon input methods to assign the following parameters to model cells:

- Reservoir Number I_{RES} $[-]$,
- Land surface elevation of the reservoir B_{RES} $[L]$,
- Vertical hydraulic conductivity of the reservoir bed HC_{RES} $[LT^{-1}]$,
- Thickness of the reservoir bed R_b $[L]$
- Layer Indicator $IRESL$ $[-]$
- Parameter Number $[-]$ Parameter Number is used to group cells, where the HC_{RES} values are to be estimated by the parameter estimation programs PEST (Section 2.6.8) or MODFLOW-2000 (Section 2.6.7). Refer to the corresponding sections for parameter estimation steps.

The water table elevations of reservoirs are specified in the Stage-Time Table of Reservoirs dialog box (see below). The land surface elevation within the specified area of potential inundation for each reservoir is typically defined by the average land surface elevation of individual cells within the area. At cells in which reservoir stage exceeds land surface elevation within the specified reservoir area, the reservoir boundary is activated. Similarly, wherever reservoir stage is less than the land surface elevation of a cell, the reservoir boundary is not activated. If reservoir stage

drops below the lowest land surface elevation for all cells within the specified reservoir area, water exchange is not simulated between the reservoir and the underlying groundwater system.

In active cells, water exchange between surface water and groundwater is computed in a manner identical to the River package (see Section 2.6.1.8). The Reservoir package is ideally suited for cases where leakage from or to reservoirs may be a significant component of flow in a groundwater system; however, if reservoir stage is unknown, then a more complex conceptualization would be needed in which reservoir stage would be computed as part of the simulation rather than having stage specified as model input. Programs that compute the lake stages based on inflows and outflows exist, for example Cheng and Anderson [16] or Council [29].

Three options are available for simulating leakage between a reservoir and the underlying groundwater system. The first option simulates leakage only to layer 1; the second option simulates leakage to the uppermost active cell; and the third option simulates leakage to a specified layer for each active reservoir cell. Inherent in the simulation of reservoirs is that the reservoir only partially penetrates an active model cell. If the reservoir fully penetrates a cell, the reservoir leakage will be simulated in a lower cell. Thus, water exchange between the groundwater system and the reservoir takes place across the bottom of the reservoir and the top of the model cells.

Leakage between the reservoir and the underlying groundwater system is simulated for each model cell corresponding to the inundated area by multiplying the head difference between the reservoir and the groundwater system by the hydraulic conductance of the reservoir bed. Equation 2.16 defines the hydraulic conductance of the reservoir bed.

$$C_{RES} = HC_{RES} \cdot DELC(I) \cdot DELR(J)/R_b \tag{2.16}$$

where $DELC(I)$ is the width of the model row I, $DELR(J)$ is the width of the model column J.

Reservoir bed thickness is subtracted from the land surface elevation of the reservoir to obtain the elevation of the base of the reservoir bed sediments. The elevation of the base of the reservoir bed sediments is used in computing leakage. When the hydraulic head in the groundwater system is above the base of the reservoir bed sediments, leakage Q_{RES} $[L^3T^{-1}]$ from or to the groundwater system is computed by equation 2.17.

$$Q_{RES} = C_{RES} \cdot (H_{RES} - h) \tag{2.17}$$

where H_{RES} is the reservoir stage $[L]$ and h is the hydraulic head in the aquifer underlying the reservoir $[L]$. When the hydraulic head is lower than the elevation of the base of the reservoir bed sediments (H_{RESBOT}), leakage from the reservoir to the groundwater system is computed by:

$$Q_{RES} = C_{RES} \cdot (H_{RES} - H_{RESBOT}) \tag{2.18}$$

► To specify the water table elevations (stages) of reservoirs

1. Click the Stage button from the Reservoir Package dialog box (Fig. 2.23).
   A Stage-Time Table of Reservoirs dialog box appears (Fig. 2.24).
2. Select a reservoir number (a row) from the first table.
   The reservoir number is corresponding to the number I_{RES} (see above). The description column is a place for the user to take notes.
3. Type the observation time and the corresponding stage into the second table.
   The observation time is measured from the start of the model simulation, to which the measured stage pertains.

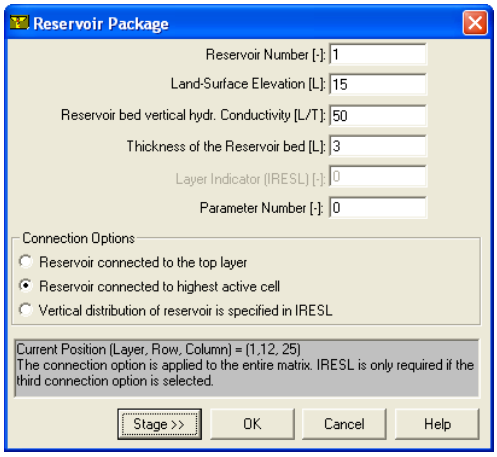

Reservoir Package
Reservoir Number [-]: 1
Land-Surface Elevation [L]: 15
Reservoir bed vertical hydr. Conductivity [L/T]: 50
Thickness of the Reservoir bed [L]: 3
Layer Indicator (IRESL) [-]: 0
Parameter Number [-]: 0
Connection Options
Reservoir connected to the top layer
Reservoir connected to highest active cell
Vertical distribution of reservoir is specified in IRESL
Current Position (Layer, Row, Column) = (1,12, 25)
The connection option is applied to the entire matrix. IRESL is only required if the third connection option is selected.
Stage >>
OK
Cancel
Help

Fig. 2.23. The Reservoir Package dialog box

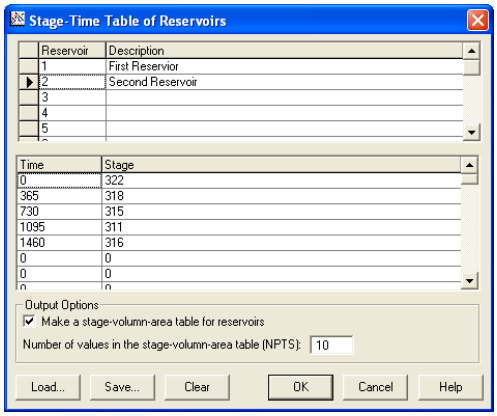


Fig. 2.24. The Stage-Time Table of Reservoirs dialog box

The Reservoir package requires the input of the starting and ending stages for each stress period. These stage values are linearly interpolated to the beginning of each time step to determine whether the reservoir boundary is activated at that time point. The stage values for each stress period are obtained by linear interpolation using the values specified in the Stage-Time Table of Reservoirs dialog box. If the starting time of a stress period is earlier than the earliest observation time in the table, the earliest observed stage is used as the starting stage for that stress period. Similarly, if the ending ending time of a stress period is beyond the latest observation time, the latest observed stage is used.

► Output Option

1. *Make a stage-volume-area table for reservoirs.*: If this option is checked, reservoir stage, area, and volume will be printed to the Run Listing File of MODFLOW each time step.
2. *Number of values in the stage-volume-area table (NPTS)*: NPTS is the number of values in printed table of stage, volume, and area for each reservoir. First and last stage value are minimum and maximum elevations within area of potential inundation. A value of 15 or greater is recommended for detailed representation of stage-volume and stage-area relations.

2.6.1.8 MODFLOW | Flow Packages | River

The purpose of the River package is to simulate the effect of flow between groundwater systems and surface-water features, such as rivers, lakes or reservoirs.

Using the Data Editor, a river is defined by using the Cell-by-Cell or Polygon input methods to assign parameters to model cells or by using the Polyline input method and assigning parameters to vertices of the polylines along the trace of the river. The input parameters are assumed to be constant during a given stress period. For transient flow simulations involving several stress periods, the input parameters can be different from period to period. The input methods require different parameters as described below.

- When using the Polyline input method, right-click on a vertex to specify its properties in the River Parameters dialog box (Fig. 2.25). If the properties are assigned to one vertex only, the properties of all vertices of the polyline are assumed to be the same. The settings of the dialog box are described below.
  - *Layer Option* and *Layer Number*: Layer Option controls how the layer number of a river is determined.
    * If Layer Option is "Assign layer number manually", the value of *Layer Number* defines the model layer number for all model cells downstream from a vertex until the next vertex redefines the layer number.
    * If Layer Option is "Assign layer number automatically", the river is assigned to a layer where the elevation of the riverbed bottom B_{riv} (see below) is located between the top and bottom of the layer. The layer number

is set to 1 if B_{riv} is higher than the top of the first layer. The layer number is set to the last layer if R_{BOT} is lower than the bottom of the last layer.

- Active: Check this box to activate a vertex. Clear the Active box to deactivate a vertex. The properties of an active vertex will be used in the simulation. The properties of an inactive vertex are ignored.
- *Hydraulic Conductivity of Riverbed (K_{riv}) [LT^{-1}]*, *Head in the river (H_{riv}) [L]*, *Elevation of the Riverbed bottom (B_{riv}) [L]*, *Width of the river (W_{riv}) [L]*, and *Thickness of the riverbed (M_{riv}) [L]*: The value K_{riv} describes all of the head loss between the river and the aquifer. It depends on the material and characteristics of the riverbed itself and the immediate environment. Since the river package requires the input of H_{riv}, B_{riv}, and river hydraulic conductance (C_{RIV}) to each cell of a river, the input values K_{riv}, H_{riv} and B_{riv} at active vertices are linearly interpolated or extrapolated to each cell along the trace of the polyline and the value C_{riv} is obtained by

$$C_{riv} = \frac{K_{riv} \cdot L \cdot W_{riv}}{M_{riv}} \tag{2.19}$$

  where L is the length of the river within a cell.
- *Parameter Number [$-$]*: Since C_{riv} is usually unknown, it must be estimated. Parameter Number is used to group cells, where the C_{riv} values are to be estimated by the parameter estimation programs PEST (Section 2.6.8) or MODFLOW-2000 (Section 2.6.7). Refer to the corresponding sections for parameter estimation steps. The value of Parameter Number is assigned to all model cells downstream from a vertex until the next vertex redefines the parameter number.
- *Density of River Fluid [M/L^3]*: This value represents the prescribed density of fluid entering the groundwater system from the river. This value is used by SEAWAT only if it is running in a *uncoupled mode*, i.e., the density-effect of

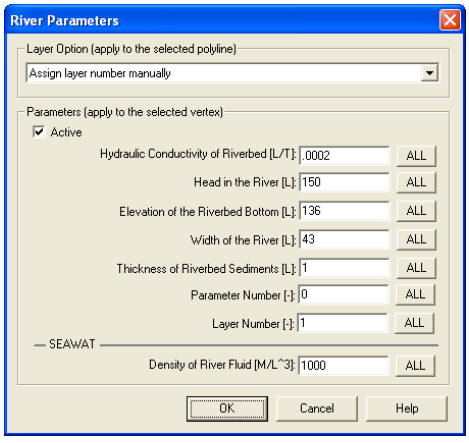


Fig. 2.25. The River Parameters dialog box

all species are turned off (see 2.6.2.1) and the *Density of river fluid* options in the Simulation Settings (MT3TMS/SEAWAT) dialog box (see Fig. 2.46 on p. 89) is set as *User-Specified in the River Package*.
  - The ALL button: Click the ALL button of a property to copy the property value to all other active vertices.
- When using the Cell-by-cell or Polygon input methods, the following values are to be assigned to model cells of a river. See the explanations above for the definition of the input values.
  - *Hydraulic Conductance of the riverbed (C_{riv}) [L^2T^{-1}]*
  - *Head in the river (H_{riv}) [L]*,
  - *Elevation of the Riverbed bottom (B_{riv}) [L]*,
  - *Parameter Number [$-$]*,
  - *Thickness of the riverbed (M_{riv}) [L]*, and
  - *Density of River Fluid [M/L^3]*

In a model cell containing river parameters, the flow rate Q_{riv} between the river and groundwater is calculated by equations 2.20 and 2.21. By default, MODFLOW saves the calculated flow rates in the BUDGET.DAT, which can be used for water balance calculations. If the groundwater hydraulic head (h) is greater than R_{BOT}, the leakage rate Q_{RIV} from the river to the aquifer is calculated by

$$Q_{riv} = C_{riv} \cdot (h_{riv} - h) \qquad \text{if} \qquad h > B_{riv} \qquad (2.20)$$

The value of Q_{RIV} is negative if the hydraulic head h is greater than H_{RIV}. It means that water flows from the aquifer into the river and is removed from the groundwater system. When h falls below the bottom of the riverbed, the leakage rate through the riverbed is given by

$$Q_{riv} = C_{riv} \cdot (h_{riv} - B_{riv}) \qquad \text{if} \qquad h < B_{riv} \qquad (2.21)$$

2.6.1.9 MODFLOW | Flow Packages | Streamflow-Routing

The Streamflow-Routing (STR) package (Prudic [98]) is designed to account for the amount of flow in streams and to simulate the interaction between surface streams and groundwater. Streams are divided into segments and reaches. Each reach corresponds to individual cells in the finite-difference grid. A segment consists of a group of reaches connected in downstream order. Streamflow is accounted for by specifying flow for the first reach in each segment, and then computing stream-flow to adjacent downstream reaches in each segment as inflow in the upstream reach plus or minus leakage from or to the aquifer in the upstream reach. The accounting scheme used in this package assumes that streamflow entering the modelled reach is instantly available to downstream reaches. This assumption is generally reasonable because of the relatively slow rates of groundwater flow.

Streamflow into a segment that is formed from tributary streams is computed by adding the outflows from the last reach in each of the specified tributary segments. If a segment is a diversion, then the specified flow into the first reach of the segment

is subtracted from flow in the main stream. However, if the specified flow of the diversion is greater than the flow out of the segment from which flow is to be diverted then no flow is diverted from that segment.

Using the Data Editor, a stream is defined by using the Cell-by-Cell or Polygon input methods to assign parameters to model cells or by using the Polyline input method and assigning parameters to vertices of the polylines along the trace of the stream. The input parameters are assumed to be constant during a given stress period. For transient flow simulations involving several stress periods, the input parameters can be different from period to period. The input methods require different parameters as described below.

- When using the Polyline input method, right-click on a vertex to specify its properties in the River Parameters dialog box (Fig. 2.26). If the properties are assigned to one vertex only, the properties of all vertices of the polyline are assumed to be the same. The settings of the dialog box are described below.

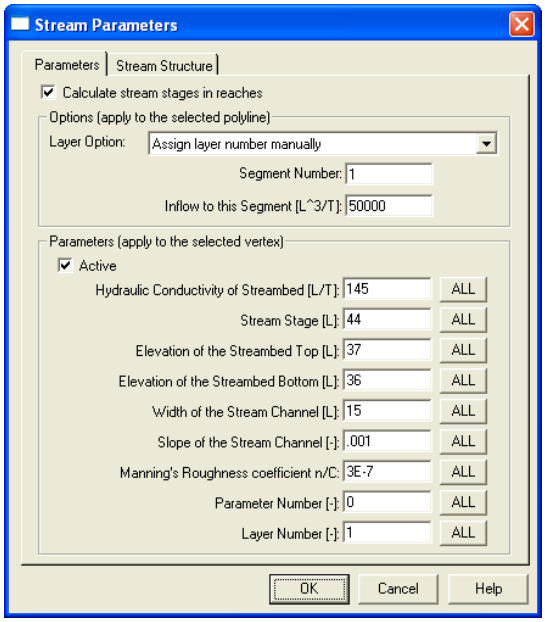


Fig. 2.26. The Stream Parameters dialog box

  - Calculate stream stages in reaches: If this option is selected, the stream water depth d_{str} in each reach is calculated from Manning's equation under the assumption of a rectangular stream channel. See equation 2.25 below.
  - Options (apply to the selected polyline):
    * Layer Option and Layer Number: Layer Option controls how the layer number of a stream reach is determined.

  - If Layer Option is "Assign layer number manually", the value of *Layer Number* defines the model layer number for all model cells downstream from a vertex until the next vertex redefines the layer number.
  - If Layer Option is "Assign layer number automatically", the river is assigned to a layer where the elevation of the Streambed bottom Bot_{str} (see below) is located between the top and bottom of the layer. The layer number is set to 1 if Bot_{str} is higher than the top of the first layer. The layer number is set to the last layer if Bot_{str} is lower than the bottom of the last layer.
* Segment Number is a number assigned to a polyline. Segments must be numbered in downstream order. The maximum number allowed is 1000.
* Inflow to this Segment [L^3T^{-1}] is the streamflow entering a segment (polyline). When inflow into a segment is the sum of outflow from a specified number of tributary segments, the segment inflow values are specified as -1.

– Parameters (apply to the selected vertex):
* Active: Check this box to activate a vertex. Clear the Active box to deactivate a vertex. The input parameters at active vertices are linearly interpolated or extrapolated to each cell along the trace of the polyline and used in the simulation. The parameters of an inactive vertex are ignored.
* Hydraulic Conductivity of Streambed (K_{str}) [LT^{-1}], Width of the Stream Channel (W_{str}) [L], Elevation of the Streambed Top (Top_{str}) [L], and Elevation of the Streambed Bottom (Bot_{str}) [L]: The value K_{str} describes all of the head loss between the stream and the aquifer. It depends on the material and characteristics of the streambed itself and the immediate environment. Since the STR package requires the input of stream hydraulic conductance (C_{str}) to each reach of a stream, the input parameters at active vertices are linearly interpolated or extrapolated to each cell along the trace of the polyline and C_{str} is obtained by

$$C_{str} = \frac{K_{str} \cdot L \cdot W_{str}}{Top_{str} - Bot_{str}} \tag{2.22}$$

  where L is the length of the stream within a cell.
* Stream Stage (h_s) [L] is the head in the stream. In a model cell containing a stream reach, the leakage rate Q_{str} between the reach and groundwater is calculated by equations 2.23 and 2.24. By default, MODFLOW saves the calculated leakage rates in the BUDGET.DAT, which can be used for water balance calculations.

$$Q_{str} = C_{str} \cdot (h_s - h) \qquad \text{if} \qquad h > Bot_{str} \tag{2.23}$$

$$Q_{str} = C_{str} \cdot (h_s - Bot_{str}) \qquad \text{if} \qquad h \leq Bot_{str} \tag{2.24}$$

* Slope of the Streambed Channel (S_{str}) [$-$] and Manning's roughness coeff. n/C: These parameters are used only when the option Calculate

stream stages in reaches is selected. To obtain the stream stage, the stream water depth (d_{str}) is calculated using the Manning's equation under the assumption of a rectangular stream channel. The calculated water depth is added to the streambed top to get the stream stage.
The Manning's equation for a rectangular stream channel is

$$d_{str} = \left[\frac{Q \cdot n}{C \cdot W_{str} \cdot S_{str}^{1/2}} \right]^{3/5} \tag{2.25}$$

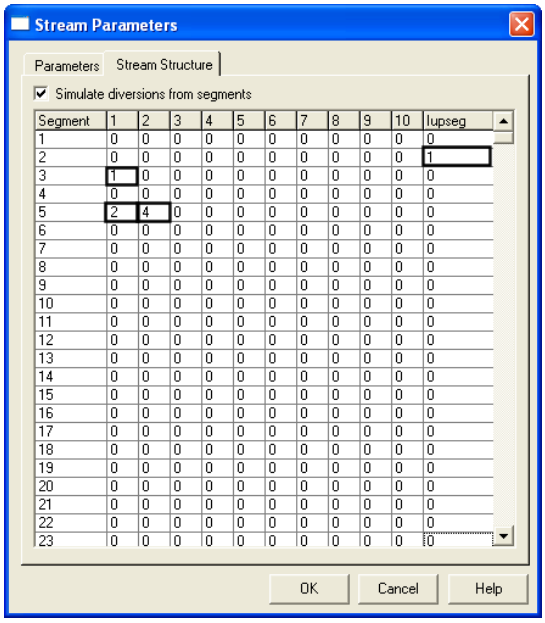
where Q $[L^3T^{-1}]$ is the calculated stream discharge, n $[-]$ is Manning's roughness coefficient, W_{str} $[L]$ is the width of the channel, and C is a conversion factor, which depends on the length and time units of the model:

$$\begin{aligned} C &= 1 \left[\frac{m^{1/3}}{s} \right] = 86400 \left[\frac{m^{1/3}}{day} \right] \\ &= 1.486 \left[\frac{ft^{1/3}}{s} \right] = 128383 \left[\frac{ft^{1/3}}{day} \right] \end{aligned} \tag{2.26}$$

Although n and C appear separately in equation 2.25, only the values of n/C or C/n are used in the computer code. The user needs therefore only to specify the value of n/C. Some of the experimental values of the Manning's roughness coefficient can be found in the documentation of the STR package [98].

* Parameter Number $[-]$: Since C_{str} is usually unknown, it needs to be estimated. Parameter Number is used to group cells, where the C_{str} values are to be estimated by the parameter estimation programs PEST (Section 2.6.8) or MODFLOW-2000 (Section 2.6.7). Refer to the corresponding sections for parameter estimation steps. The value of Parameter Number is assigned to all model cells downstream from a vertex until the next vertex redefines the parameter number.
* The ALL button: Click the ALL button of a property to copy the property value to all other active vertices.

– *Stream Structure* describes the configuration of a stream system. Each row in the table (Fig. 2.27) represents a stream segment in the model. Each segment can have up to 10 tributary segments. The numbers of the tributary segments are specified in the columns 1 to 10. The column Iupseg is the number of the upstream segment from which water is diverted. For a segment that is not a diversion, Iupseg must be specified as zero. Iupseg is used only when the option Simulate diversions from segments is checked. The values in Fig. 2.27 indicate that segment 2 is diverted from segment 1, segment 1 is a tributary segment of segment 3, and segments 2 and 4 are tributary segments of segment 5. The configuration of the stream system is shown in Fig. 2.28.



Segment	1	2	3	4	5	6	7	8	9	10	Iupseg
1	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	1
3	1	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0	0
5	2	4	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0	0	0	0	0
22	0	0	0	0	0	0	0	0	0	0	0
23	0	0	0	0	0	0	0	0	0	0	0

Fig. 2.27. Specification of the stream structure

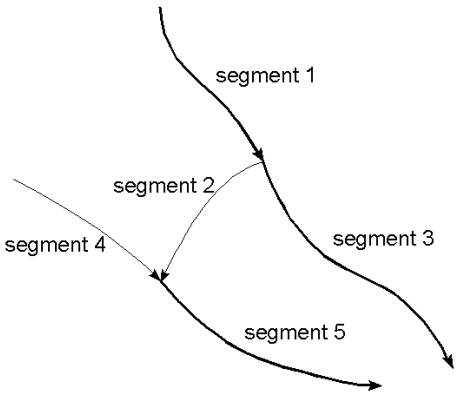


Fig. 2.28. The stream system configured by the table of Fig. 2.27

- When using the Cell-by-cell or Polygon input methods, the following values are to be assigned to model cells alone the trace of a stream. See the explanations above for the definition of the input values.
  - Segment Number.
  - Inflow to this Segment [L^3T^{-1}].
  - Reach Number is a sequential number in a segment that begins with one for the farthest upstream reach and continues in downstream order to the last reach in the segment. Using the Cell-by-cell or Polygon methods only one

reach can be assigned to a model cell, although the STR package allows the user to assign more than one reach in different segments to the same model cell.
- Stream Stage (h_s) [L].
- Streambed Hydraulic Conductance (C_{str}) [L^2T^{-1}].
- Elevation of the Streambed Top (TOP_{str}) [L].
- Elevation of the Streambed Bottom (BOT_{str}) [L].
- Width of the Stream Channel (W_{str}) [L].
- Slope of the Streambed Channel (S_{tr}) [$-$].
- Manning's roughness coeff. n/C.
- Parameter Number [$-$]

2.6.1.10 MODFLOW | Flow Packages | Time-Variant Specified-Head

For transient simulations, the Time-Variant Specified-Head package [78] allows constant head cells to take on different head values for each time step.

A time-variant specified head boundary is defined by using the Cell-by-Cell or Polygon input methods of the Data Editor to assign the following parameters to model cells:

- *Flag [−].* A non-zero value indicates that a cell is specified as a time-variant specified-head boundary.
- *Start Head h_s [L].* This value is the prescribed hydraulic head of a cell at the start of the stress period.
- *End Head h_e [L].* This value is the prescribed hydraulic head of a cell for the last time step of a stress period.

This package does not alter the way contant head boundaries are formulated in the finite-difference equations of MODFLOW. It simply sets the element in the IBOUND array to a negative value for all cells where a time-variant specified-head boundary is selected ($Flag \neq 0$). For each time step within a period, the package linearly interpolates prescribed hydraulic heads h for each time-variant specified-head boundary cell by using the equation:

$$h = h_s + (h_e - h_s) \cdot \frac{PERTIM}{PERLEN} \tag{2.27}$$

where $PERTIM$ is the starting time of a time step within a stress period and $PERLEN$ is the length of the stress period. The interpolated head values remain constant during a time step. If a cell is specified as a time-variant specified-head boundary for a stress period and omitted in the specification for a subsequent period, it remains a fixed-head boundary with a head equal to that at the end of the previous period.

2.6.1.11 MODFLOW | Flow Packages | Well

An injection or a pumping well is defined by using the Cell-by-Cell or Polygon input methods of the Data Editor to assign the following parameters to model cells. The input parameters are assumed to be constant during a given stress period. For transient flow simulations involving several stress periods, the input parameters can be different from period to period.

- *Recharge rate of the well (Q_w) [L^3T^{-1}]*. Negative values are used to indicate pumping wells, while positive cell values indicate injection wells. The injection or pumping rate of a well is independent of both the cell area and the hydraulic head in the cell. MODFLOW assumes that a well penetrates the full thickness of the cell. To simulate wells that penetrate more than one model layer, the injection or pumping rate for each layer has to be specified. The total injection or pumping rate for a multi-layer well is equal to the sum of those from the individual layers. For confined layers, the injection or pumping rate for each layer (Q_k) can be approximately calculated by dividing the total rate (Q_{total}) in proportion to the layer transmissivities (McDonald and Harbaugh [85]):

$$Q_k = Q_{total} \cdot \frac{T_k}{\Sigma T} \tag{2.28}$$

  where T_k is the transmissivity of layer k and ΣT is the sum of the transmissivity values of all layers penetrated by the multi-layer well. Another possibility to simulate a multi-layer well is to set a very large vertical hydraulic conductivity (or vertical leakance), e.g. 1 m/s, to all cells of the well. The total pumping rate is then assigned to the lowest cell of the well. For display purposes, a very small pumping rate (say, $-1 \times 10^{-10} m^3/s$) can be assigned to other cells of the well. In this way, the exact extraction rate from each penetrated layer can be obtained by using the Water Budget Calculator. See Section 4.1.2.5 for how to calculate subregional water budget.
- *Parameter Number [−]*: Parameter Number is used to group cells, where the Q_w values are to be estimated by the parameter estimation programs PEST (Section 2.6.8) or MODFLOW-2000 (Section 2.6.7). Refer to the corresponding sections for parameter estimation steps.
- *Density of Injection Fluid [M/L^3]*: This value is used by SEAWAT only if it is running in a *uncoupled mode*, i.e., the density-effect of all species are turned off (see 2.6.2.1) and the *Density of Injection Well Fluid* options in the Simulation Settings (MT3TMS/SEAWAT) dialog box (see Fig. 2.46 on p. 89) is set as *User-Specified in the Well Package*.

2.6.1.12 MODFLOW | Flow Packages | Wetting Capability

The wetting capability of the Block-Centered Flow 2 (BCF2) package [86] allows the simulation of a rising water table into unsaturated (dry) model layers.

The BCF2 package is identical to the BCF1 package of MODFLOW-88 [85] except for the wetting and drying of cells. A cell falls dry when the head is below

the bottom elevation of the cell. When a cell falls dry, IBOUND is set to 0 (which indicates a no flow or an inactive cell), all conductance values to the dry cell are set to zero. No water can flow into the cell as the simulation proceeds and the cell remains inactive even if neighboring water tables rise again.

To overcome this problem, a value THRESH, called wetting threshold, is introduced to the BCF2 package (or later versions of this package). The computer code uses this value to decide, whether a dry or an inactive cell can be turned into a wet (active) cell.

- If THRESH $= 0$, the dry cell or the inactive cell cannot be wetted.
- If THRESH < 0, only the cell below the dry cell (or inactive cell) can cause the cell to become wet.
- If THRESH > 0, the cell below the dry cell (or inactive cell) and the four horizontally adjacent cells can cause the cell to become wet.

A dry cell or an inactive cell can be turned into an active cell if the head from the previous iteration in a neighboring cell is greater than or equal to the turn-on threshold TURNON.

$$TURNON = BOT + |THRESH| \tag{2.29}$$

where BOT is the elevation of the bottom of the cell.

To improve the stability of the numerical solution, a neighboring cell cannot become wet as a result of a cell that has become wet in the same iteration; only variable-head cells either immediately below or horizontally adjacent to the dry cell can cause the cell to become wet. When a cell is wetted, its IBOUND value is set to 1 (which indicates a variable-head cell), vertical conductance values are set to the original values, and the hydraulic head h at the cell is set by using one of the following equations.

$$h = BOT + WETFCT \cdot (h_n - BOT) \tag{2.30}$$

$$h = BOT + WETFCT \cdot |THRESH| \tag{2.31}$$

where h_n is the head at the neighboring cell that causes the dry cell to wet and $WETFCT$ is a user-specified constant called the wetting factor. The user may select between equations 2.30 and 2.31 in the Wetting Capability dialog box (Fig. 2.29). This dialog box appears after selecting *Models* | *MODFLOW* | *Flow Packages* | *Wetting Capability*. The dialog box allows the user to specify the iteration interval for attempting to wet cells IWETIT. Wetting is attempted every IWETIT iterations. When using the PCG2 solver [59], this applies to outer iterations and not inner iterations. The reason for adjusting IWETIT is that the wetting of cells sometimes produces erroneous head changes in neighboring cells during the succeeding iteration, which may cause erroneous conversions of those cells. Waiting a few iterations until heads have had a chance to adjust before testing for additional conversions can prevent these erroneous conversions. When setting IWETIT greater than one, there is some risk that cells may be prevented from correctly converting from dry to wet. If the solution for a time step is obtained in less than IWETIT iterations, then there

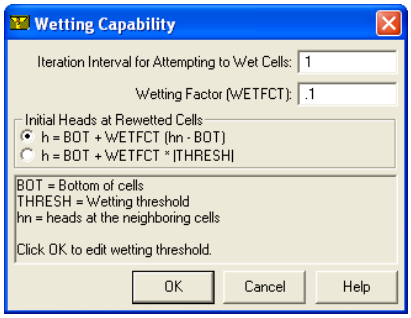

Wetting Capability
Iteration Interval for Attempting to Wet Cells: 1
Wetting Factor (WETFCT): .1
Initial Heads at Rewetted Cells
h = BOT + WETFCT (hn - BOT)
h = BOT + WETFCT * |THRESH|
BOT = Bottom of cells
THRESH = Wetting threshold
hn = heads at the neighboring cells
Click OK to edit wetting threshold.
OK
Cancel
Help

Fig. 2.29. The Wetting Capability dialog box

will be no check during that time step to see if cells should be converted from dry to wet. The potential for this problem to occur is greater in transient simulations, which frequently require only a few iterations for a time step.

The method of wetting and drying cells used in the BCF2 Package can cause problems with the convergence of the iterative solvers used in MODFLOW. Convergence problems can occur in MODFLOW even without the wetting capability but problems are more likely to occur when the wetting capability is used. Symptoms of a problem are slow convergence or divergence combined with the frequent wetting and drying of the same cells. It is normal for the same cell to con-vert between wet and dry several times during the convergence process but frequent conversions are an indication of problems. As a matter of fact, situations exist where the real solution oscillates such as in the case of a well causing a drawdown, which makes the well cells fall dry. This in turn switches off the well and leads to a rise of the water table and wetting of the well cell etc. The user can detect such situations by examining the model run record file OUTPUT.DAT; a message is printed each time a cell converts. The basic tools at hand to combat convergence problems are:

- Choose vertical discretization such that only few cells will fall dry.
- Choose wetting from below only (i.e. set THRESH<0).
- Change to a different preconditioner, if the PCG2 solver is used.
- Change to a different solver.
- Increase the modulus of THRESH.
- Increase IWETIT.
- Decrease pumping rates of wells.

2.6.1.13 MODFLOW | Solvers

To calculate heads in each cell in the finite-difference grid, MODFLOW prepares one finite difference equation for each cell, expressing the relationship between the head at a node and the heads at each of the six adjacent nodes at the end of a time step. Because each equation may involve up to seven unknown values of head, and because the set of unknown head values changes from one equation to the next through the grid, the equations for the entire grid must be solved simultaneously at each time

step. The system of simultaneous finite difference linear equations can be expressed in matrix notation as

$$\underline{A} \cdot \underline{x} = \underline{b} \tag{2.32}$$

where $\underline{A}$ is a coefficient matrix assembled by MODFLOW using user-specified model data; $\underline{b}$ is a vector of defined flows, terms associated with head-dependent boundary conditions and storage terms at each cell; $\underline{x}$ is a vector of hydraulic heads at each cell. One value of the hydraulic head for each cell is computed at the end of each time step. **PM** supports four packages (solvers) for solving systems of simultaneous linear equations:

- Direct Solution (DE45) package,
- Preconditioned Conjugate-Gradient 2 (PCG2) package,
- Strongly Implicit Procedure (SIP) package,
- Slice-Successive Over Relaxation (SSOR) package, and
- Geometric Multigrid Solver (GMG) package.

Input parameters of these solution methods are discussed below. See McDonald and Harbaugh [85], [59], Harbaugh [53], and Wilson and Naff [115] for detailed mathematical background and numerical implementation of these solvers. Various comparisons between the solution methods can be found in Trescott [112], Kuiper [75], Behie and Forsyth [14], Scandrett [106], and Hill [60]. Hill[60] indicates that the greatest differences in solver efficiency on scalar computers occur for three-dimensional, non-linear problems. For these types of problems, it may be well worth the time and effort to try more than one solver.

Note. The GMG solver [115] is only implemented in MODFLOW-2000. The MODFLOW version "MODFLOW + Density package from KIWA" does not support the Direction Solution package.

MODFLOW | Solvers | DE45

Although a direct solver requires more memory and typically requires more computational effort than iterative solvers, it may execute faster than an iterative solver in some situations. The Direct Solution package [53] uses Gaussian elimination with an alternating diagonal equation numbering scheme that is more efficient than the standard method of equation numbering. It is the most efficient when solving small, linear problems.

Use the Direct Solution (DE45) dialog box (Fig. 2.30) to specify required parameters as described below:

- *Maximum iterations (external or internal)* is the maximum number of iterations in each time step. Set this number to 1 if iteration is not desired. Ideally iteration would not be required for direct solution; however, it is necessary to iterate if the flow equation is non-linear (see Problem type below) or if computer precision limitations result in inaccurate calculations as indicated by a large water budget error. For a non linear flow equation, each iteration is equally time consuming because the coefficient matrix $\underline{A}$ is changed with each iteration and Gaussian elimination is required after each change. This is called external iteration. For a linear equation, iteration is significantly faster because $\underline{A}$ is changed at most once per time step; Thus, Gaussian elimination is required at most once per time step. This is called internal iteration.
- *Max. equations in upper part of [A]*: This is the maximum number of equations in the upper part of the equations to be solved. This value impacts the amount of memory used by the solver. If specified as 0, the program will calculate the value as half the number of cells in the model, which is an upper limit. The actual number of equations in the upper part will be less than half the number of cells whenever there are no flow and constant head cells because flow equations are

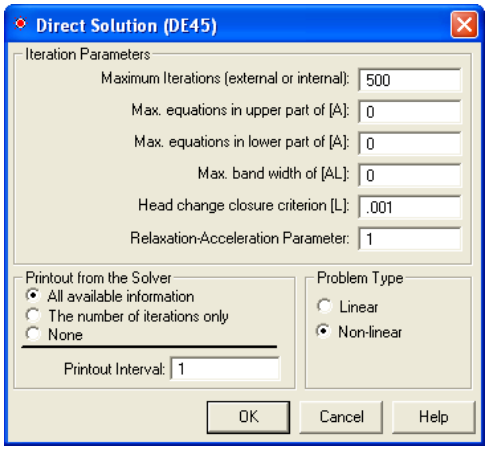


Fig. 2.30. The Direct Solution (DE45) dialog box

not formulated for these cells. The solver prints the actual number of equations in the upper part when it runs. The printed value can be used in future runs in order to minimize memory usage.

- *Max. equations in lower part of [A]*: This is the maximum number of equations in the lower part of the equations to be solved. This value impacts the amount of memory used by the solver. If specified as 0, the program will calculate the value as half the number of cells in the model, which is an upper limit. The actual number of equations in the lower part will be less than half the number of cells whenever there are no flow and constant head cells be-cause flow equations are not formulated for these cells. The solver prints the actual number of equations in the lower part when it runs. The printed value can be used in future runs in order to minimize memory usage.
- *Max. band width of AL*: This value impacts the amount of memory used by the solver. If specified as 0, the program will calculate the value as the product of the two smallest grid dimensions, which is an upper limit.
- *Head change closure criterion [L]*: If iterating, iteration stops when the absolute value of head change at every node is less than or equal to this value. The criterion is not used when not iterating, but a value must always be specified.
- *Relaxation-Accelleration Parameter (ACCL)*: ACCL is a multiplier for the computed head change for each iteration. Normally this value is 1. A value greater than 1 may be useful for improving the rate of convergence when using external iteration to solve non-linear problems. ACCL should always be 1 for linear problems. When Maximum Iterations = 1, ACCL is changed to 1 regardless of the input value.
- *Printout From the Solver*: If the option All available information is selected, the maximum head change and residual (positive or negative) are saved in the run listing file OUTPUT.DAT for each iteration of a time step whenever the time step is an even multiple of Printout Interval. If the option *The number of iterations only* is checked, the printout of maximum head change and residual is suppressed. Select the option *None* to suppress all printout from the solver. A positive integer is required by Printout Interval.
- *Problem Type*: The choice of problem type affects the efficiency of solution; significant work can be avoided if it is known that A remains constant all or part of the time.
  - *Linear* indicates that the flow equations are linear. To meet the linearity requirement, all model layers must be confined, and there must be no formulations that change based upon head (such as seepage from a river changing from head dependent flow to a constant flow when head drops below the bottom of the riverbed). Examples of non-linearity are cases with riverbed conductance, drain conductance, maximum evapotranspiration rate, evapotranspiration extinction depth, general head boundary conductance and reservoirbed conductance.
  - *Nonlinear* indicates that a non-linear flow equation is being solved, which means that some terms in $\underline{A}$ depend on simulated head. Example of head dependent terms in $\underline{A}$ are transmissivity for water-table layers, which is based

on the saturated thickness; flow terms for rivers, drains, and evapotranspiration convert between head dependent flow and constant flow; and the change in storage coefficient when a cell converts between confined and unconfined. When a non-linear flow equation is being solved, external iteration is normally required in order to accurately approximate the non-linearities. Note that when non-linearities caused by water table calculations are part of a simulation, there are not necessarily any obvious signs in the output from a simulation that does not use external iteration to indicate that iteration is needed. In particular, the budget error may be acceptably small without iteration even though there is significant error in head because of non-linearity. To understand this, consider the water table correction for transmissivity. For each iteration a new transmissivity value is calculated based on the previous head. Then the flow equations are solved, and a budget is computed using the new head with the same transmissivities. No budget discrepancy results because heads are correct for the transmissivity being used at this point; however, the new heads may cause a significant change in transmissivity. The new transmissivity will not be calculated unless there is another iteration. Therefore, when one or more layers are under water table conditions, iteration should always be tried. The maximum change in head during each iteration (printed by the solver) provides an indication of the impact of all non-linearities.

MODFLOW | Solvers | PCG2

The required parameters for the PCG2 package are specified in the Preconditioned Conjugate-Gradient Package 2 dialog box (Fig. 2.31). They are described below:

- *Preconditioning Method*: The PCG2 package provides two preconditioning options: the modified incomplete Cholesky preconditioner MICCG [10] and the

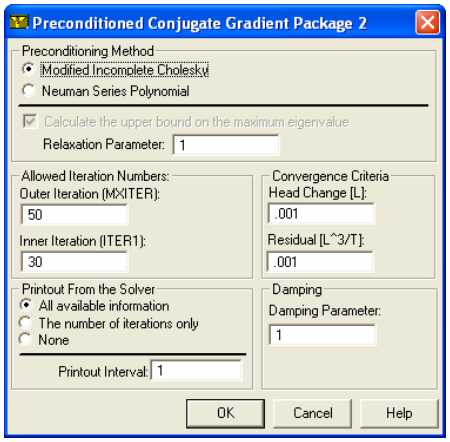


Fig. 2.31. The Preconditioned Conjugate Gradient Package 2 dialog box

Neuman Series Polynomial preconditioner POLCG [105].

- *Relaxation Parameter* is used with MICCG. Usually, this parameter is equal to 1. Ashcraft and Grimes [9] found out that for some problems a value of 0.99, 0.98 or 0.97 would reduce the number of iterations required for convergence.
- The option *Calculate the upper bound on the maximum eigenvalue* is only available when POLCG is selected. Check this box, if the solver should calculate the upper bound on the maximum eigenvalue of $\underline{A}$. Otherwise, a value of 2 will be used. The upper bound is estimated as the largest sum of the absolute values of the components in any row of $\underline{A}$. Estimation of the upper bound uses slightly more execution time per iteration.
- *Allowed Iteration Numbers*:
  - *MXITER* is the maximum number of outer iterations. For each outer iteration, $\underline{A}$ and $\underline{b}$ (equation 2.32) are updated by using the newly calculated hydraulic heads. For a linear problem, MXITER should be 1, unless more that ITER1 inner iterations are required. A larger number (generally less than 100) is required for a nonlinear problem. Outer iterations continue until the final convergence criteria (see below) are met on the first inner iteration.
  - *ITER1* is the maximum number of inner iterations. Equation 2.32 with a new set of $\underline{A}$ and $\underline{b}$ is solved in inner iterations. The inner iterations continue until ITER1 - iterations are executed or the final convergence criteria (see below) are met.
- *Convergence Criteria*:
  - *Head Change* $[L]$ is the head change criterion for convergence. When the maximum absolute value of the head change at all nodes during an iteration is less than or equal to the specified Head Change, and the criterion for Residual is satisfied (see below), iteration stops.
  - *Residual* $[L^3T^{-1}]$ is the residual criterion for convergence. Residual is calculated as $\underline{A} \cdot \underline{x} - \underline{b}$ for each inner iteration. When the maximum absolute value of the residual at all cells during an iteration is less than or equal to Residual, and the criterion for Head Change is satisfied (see above), iteration stops.
- *Printout From the Solver*: Printout Interval requires a positive integer. If the option All available information is selected, the maximum head change and residual (positive or negative) are saved in the run listing file OUTPUT.DAT for each iteration of a time step whenever the time step is an even multiple of *Printout Interval*. If the option *The number of iterations only* is checked, the printout of maximum head change and residual is suppressed. Select the option *None* to suppress all printout from the solver.
- *Damping Parameter*: The Damping Parameter is a multiplier for the computed head change for each iteration. Normally this value is 1. A value smaller than 1 may be useful for unstable systems.

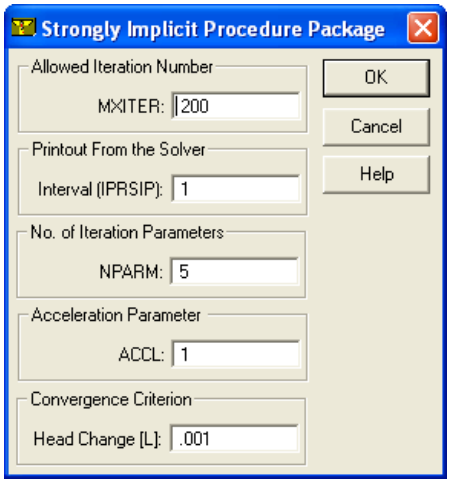


Fig. 2.32. The Strongly Implicit Procedure Package dialog box

MODFLOW | Solvers | SIP

The required parameters for the SIP package are specified in the Strongly Implicit Procedure Package dialog box (Fig. 2.32). The parameters are described below:

- *MXITER* is the maximum number of iterations in one time step in an attempt to solve the system of finite-difference equations.
- *IPRSIP* is the printout interval for this package. A positive integer is required. The maximum head change (positive or negative) is saved in the run record file OUTPUT.DAT for each iteration of a time step whenever the time step is an even multiple of IPRSIP. This printout also occurs at the end of each stress period regardless of the value of IPRSIP.
- *NPARM* is the number of iteration parameters to be used. Five parameters are generally sufficient.
- *ACCL* is the acceleration parameter. It must be greater than zero and is generally equal to one.
- *Head Change* [*L*] is the head change criterion for convergence. When the maximum absolute value of head change from all cells during an iteration is less than or equal to Head Change, iteration stops.

MODFLOW | Solvers | SSOR

The required parameters for SSOR package are specified in the Slice Successive Overrelaxation Package dialog box (Fig. 2.33). The parameters are described below:

- *MXITER* is the maximum number of iterations in one time step in an attempt to solve the system of finite-difference equations.

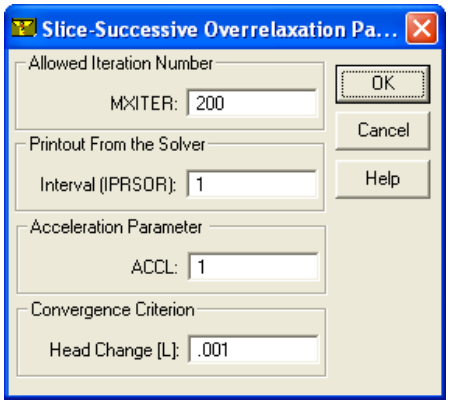


Fig. 2.33. The Slice-Successive Overrelaxation Package dialog box

- *IPRSOR* is the printout interval for SSOR. A positive integer is required. The maximum head change (positive or negative) is saved in the run record file OUTPUT.DAT for each iteration of a time step whenever the time step is an even multiple of *IPRSOR*. This printout also occurs at the end of each stress period regardless of the value of *IPRSOR*.
- *ACCL* is the acceleration parameter, usually between 1.0 and 2.0.
- *Head Change* is the head change criterion for convergence. When the maximum absolute value of head change from all cells during an iteration is less than or equal to Head Change, iteration stops.

MODFLOW | Solvers | GMG (MODFLOW-2000 Only)

The required parameters for the GMG package [115] are specified in the Geometric Multigrid Solver dialog box (Figure 2.34). The parameters are described below:

- *Iteration Control*:
  - *Maximum Number of Outer Iteration (MXITER)*: MXITER is the maximum number of outer iterations. For linear problems, MXITER can be set to 1. Fornonlinear problems, MXITER needs to be larger, but rarely more than 100.
  - *Head Change Closure Criterion HCOLOSE*: HCLOSE is the head change convergence criterion for nonlinear problems. After each linear solve (inner iteration), themaximum head change is compared against HCLOSE. HCLOSE can be set to a large number for linear problems; HCLOSE is ignored if MXITER = 1.
  - *Maximum number of inner PCG-iterations (IITER)*: IITER defines the maximum number of PCG iterations for each linear solution. A value of 100 is typically sufficient. It is frequently useful to specify a smaller number for nonlinear problems so as to prevent an excessive number of inner iterations.

  - *Budget Closure Criterion RCLOSE*: RCLOSE is the residual convergence criterion for the inner iteration. The PCG algorithm computes the l2norm of the residual and compares it against RCLOSE. Typically, RCLOSE is set to the same value as HCLOSE. If RCLOSE is set too high, then additional outer iterations may be required due to the linear equation not being solved with sufficient accuracy. On the other hand, a too restrictive setting for RCLOSE for nonlinear problems may force an unnecessarily accurate linear solution. This may be alleviated with the IITER parameter or with damping.
- *Damping Control*:
  - *Damping Method*: Two damping methods are available:
    * *Fixed Damping Value*: If this method is selected, then the Damping Value (see below) is used as a constant damping parameter.
    * *Cooley's method*: If this method is selected, then the Damping Value is used for the first outer iteration (nonlinear iteration). The damping parameter is adaptively varied on the basis of the head change, using Cooley's method as described in Mehl and Hill [87], for subsequent iterations.
  - Damping value: This defines the value of the damping parameter. For linear problems, a value of 1.0 should be used. For nonlinear problems, a value less than 1.0 but greater than 0.0 may be necessary to achieve convergence. A typical value for nonlinear problems is 0.5. Damping also helps to alleviate excessive inner PCG-iterations.
- *Preconditioner Control*:
  - *Smoother Type*:

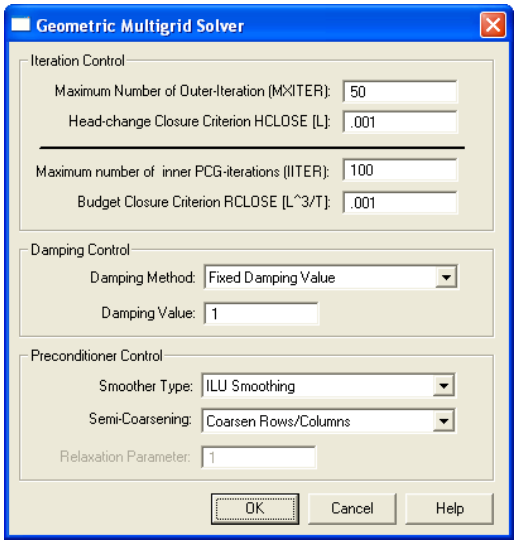


Fig. 2.34. The Geometric Multigrid Solver dialog box

  - * *ILU Smoothing*: Select this option to implement ILU(0) smoothing in the multigrid preconditioner. This smoothing requires an additional vector on each multigrid level to store the pivots in the ILU factorization.
  - * *Symmetric Gauss-Seidel (SGS) Smoothing*: Select this option to implement the Symmetric Gauss-Seidel (SGS) smoothing in the multigrid preconditioner. No additional storage is required for this smoother; users may want to use this option if available memory is exceeded or nearly exceeded when using ILU Smoothing. Using SGS smoothing is not as robust as ILU smoothing; additional iterations are likely to be required in reducing the residuals. In extreme cases, the solver may fail to converge as the residuals cannot be reduced sufficiently.
- *Semi-Coarsening*: This option controls semi-coarsening in the multigrid preconditioner. The possible options and their meanings are given as follows:
  - * *Coarsen Rows/Columns/Layers*: rows, columns and layers are all coarsened.
  - * *Coarsen Rows/Columns*: rows and columns are coarsened, but the layers are not.
  - * *Coarsen Columns/Layers*: columns and layers are coarsened, but the rows are not.
  - * *Coarsen Rows/Layers*: rows and layers are coarsened, but the columns are not.
  - * *No Coarsening*: there is no coarsening.

  Typically, the options *Coarsen Rows/Columns/Layers* or *Coarsen Rows/Columns* should be selected. In the case that there are large vertical variations in the hydraulic conductivities, then the option *Coarsen Rows/Columns* should be used. If no coarsening is implemented, the GMG solver is comparable to the PCG2 ILU(0) solver described in Hill [59] and uses the least amount of memory.
- *Relaxation Parameter*: This parameter can be used to improve the spectral condition number of the ILU preconditioned system. The value of relaxation parameter should be approximately one. However, the relaxation parameter can cause the factorization to break down. If this happens, then the GMG solver will report an assembly error and a value smaller than one for relaxation parameter should be tried. Relaxation Parameter is used only if the option *No Coarsening* is selected.

2.6.1.14 MODFLOW | Head Observations

Select *Head Observations* from the *MODFLOW* menu (or from *MODFLOW-2000 (Parameter Estimation)* or *PEST (Parameter Estimation)* menus) to specify the locations of the head observation boreholes and their associated observed (measurement) data in the Head Observations dialog box (Fig. 2.35). Using the *Save* button, the user can save the tables in separate ASCII files (see Section 6.2.6 for the formats), which can be loaded at a later time by using the *Load* button. The other options of this dialog box are described below.

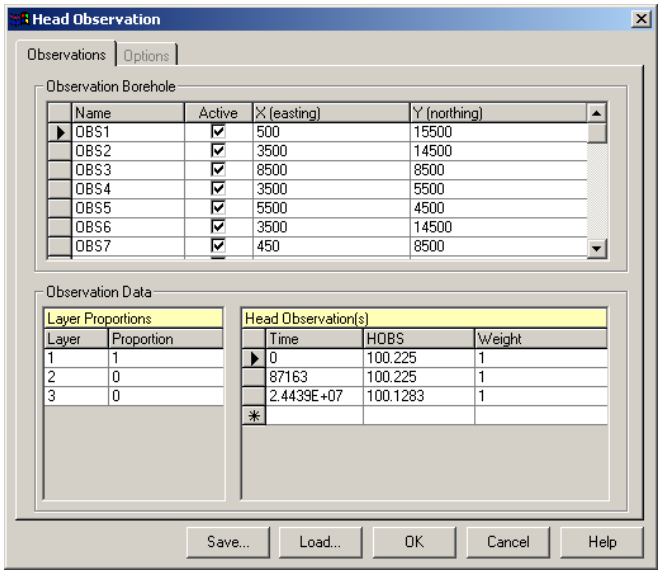


Fig. 2.35. The Head Observation dialog box

The Observations Tab

- *Observation Borehole*: The Name (OBSNAM) and the coordinates (expressed in the world coordinates according to the user-defined coordinate system) of each borehole are given in this table. The Name should be unique for each observation. A borehole is active if the Active flag is checked. To input a new borehole, scroll down to the end of the table and simply type the name and coordinates to the last (blank) row. To delete a borehole, the user selects the row to be deleted by clicking on its record selector (▭ before the first column of the table), then pressing the *Del* key.
  After a simulation, the user may select *View* | *Head Scatter Diagram* from the Modflow or PEST menus to compare the calculated and observed values. The user can also select *View* | *Head-Time Curves* of these menus to display time-series curves of both the calculated and observed values.
- The *Observation Data* group contains two tables - Layer Proportion and Head Observation(s). These tables contain the data of the selected borehole, which is marked by ▶ on the Observation Borehole table.
  - The *Layer Proportions* table: **PM** supports multi-layer observations by using this table. If an observation borehole is screened over more than one model layer, and the observed hydraulic head is affected by all screened layers, then the associated simulated value is a weighted average of the calculated hydraulic heads of the screened layers. The simulated head value h is calculated by

$$h = \frac{\sum_{i=1}^{nlay} (H_i \times PR_i)}{\sum_{i=1}^{nlay} PR_i} \tag{2.33}$$

Where nlay is the number of model layers, H_i and PR_i are the calculated head value and the proportion value of the ith layer, respectively. The proportion values generally are assigned using the thickness screened within each layer and the local hydraulic properties. A more realistic representation of this problem would be produced by calculating proportions that are based on the flow-system and hydraulic properties [63].

For a single-layer borehole, simply specify a non-zero proportion value to the layer, where the borehole is screened, and assign a proportion value of zero to all other layers. If the proportion values of all layers are zero, the observation borehole is considered as "inactive" and thus no graphical display can be generated for this borehole.

– The *Head Observation(s)* table: When specifying head observations for MOD-FLOW-2000 the third column of this table is Statistic otherwise it is *Weight*. Inserting or deleting an observation (row) is identical to the table for Observation Borehole described above.
  * *Time*: The observation time, to which the measurement pertains, is measured from the beginning of the model simulation. You may specify the observation times in any order. By clicking on the column header or the OK button, the observation times (and the associated values) will be sorted in ascending order. When calibrating a steady state flow model with one stress period, the observation time should be the length of the period. Of particular note is that when calibrating a transient flow model with PEST the observation times and the associated HOBS, Weight and Statistic values are linearly interpolated to the simulation times at the end of each stress period or time step. The interpolated values are then used for parameter estimation. When running MODFLOW-2000, the specified observation times and values are used for parameter estimation directly, without interpolation.
  * *HOBS*: The hydraulic head observed at the observation time.
  * *Weight*: The Weight of an observation gives a relative confidence level of the observed value. The higher the value, the better is the measurement. The weight can be set at zero if needed (meaning that the observation takes no part in the calculation of the objective function during a parameter estimation process), but it must not be negative. Refer to the documents of PEST [33][34][36] for the function of weights in the parameter estimation process.
  * *Statistic*: MODFLOW-2000 reads statistics from which the weights are calculated. The physical meaning of Statistic is controlled by the Options tab (see below).

The Options Tab

This tab is only used by MODFLOW-2000 for parameter estimation. There are two options:

- *Parameter Estimation Option*: When the option ”temporal changes in hydraulic heads are used as observations” is selected, the temporal change is calculated as a specified hydraulic head minus the first hydraulic head specified for that location. The first hydraulic head at a location is included in the regression. The advantage of matching temporal changes in hydraulic head is that errors that are constant in time, such as well elevation, are expunged [63].
- *Statistic Option*: This option defines the physical meaning of *Statistic* specified in the Head Observation(s) table. It also defines how the weights are calculated. Refer to Hill [62] for more details about the role of statistics and weights in solving regression problems.

Note. The PEST interface of **PM** can only handle single-layer observation boreholes. Multilayer boreholes are ignored when using PEST. However, multilayer boreholes will be used when using PEST-ASP+MODFLOW-2000.

2.6.1.15 MODFLOW | Drawdown Observations

Select *Drawdown Observations* from the *MODFLOW* menu (or from the *PEST* menu) to specify the locations of the drawdown observation boreholes and their associated observed (measurement) data in a Drawdown Observations dialog box. Its use is identical to the Head Observation dialog box. The only difference is that the head observations are replaced by drawdown observations.

Note that MODFLOW-2000 does not use drawdown observations for parameter estimation. Instead, the temporal changes in specified hydraulic heads are used.

2.6.1.16 MODFLOW | Subsidence Observations

Select this menu item to open a Subsidence Observation dialog box. Except the Layer Proportion table, the use of this dialog box is identical to the Head Observation dialog box. The Layer Proportions table is not used here, because the subsidence is the sum of the compactions in all model layers.

The specified subsidence values are solely for display purposes and not used by PEST or MODFLOW-2000 for parameter estimation.

2.6.1.17 MODFLOW | Compaction Observations

Select this menu item to open a Compaction Observation dialog box. The use of this dialog box is identical to the Head Observation dialog box, except the Layer Proportion table. The layer Proportions values are used as a flag here. When displaying compaction-time curves or a compaction scatter diagram, the sum of the compaction

values of the layers, which have a positive layer proportion value, is assign to the observation borehole.

The specified compaction values are solely for display purposes and not used by PEST or MODFLOW-2000 for parameter estimation.

2.6.1.18 MODFLOW | Output Control

The primary output file of MODFLOW is the run listing file OUTPUT.DAT. MODFLOW calculates a volumetric water budget for the entire model at the end of each time step, and saves it in the run listing file. The volumetric water budget provides an indication of the overall acceptability of the numerical solution. In numerical solution techniques, the system of equations solved by a model actually consists of a flow continuity statement for each model cell. Continuity should therefore also exist for the total flows into and out of the entire model or a sub-region. This means that the difference between total inflow and total outflow should equal the total change in storage. It is recommended to read the listing file by selecting *Models* | *Modflow* | *View* | *Run Listing File*. The run listing file also contains other essential information. In case of difficulties, this supplementary information could be very helpful. If the computational accuracy is inadequate decrease the convergence criterion in the selected solver.

In addition to the run listing file, various simulation results can be saved by checking the corresponding output terms in the MODFLOW Output Control dialog box (Fig. 2.36). The settings are described below.

- *Output Terms*: The output terms and the corresponding result files are described below. All result files are saved in the folder in which the model data are saved.
  - *Hydraulic Heads* are the primary result of a MODFLOW simulation. Hydraulic heads in each finite-difference cell are saved in the unformatted (binary) file HEADS.DAT.

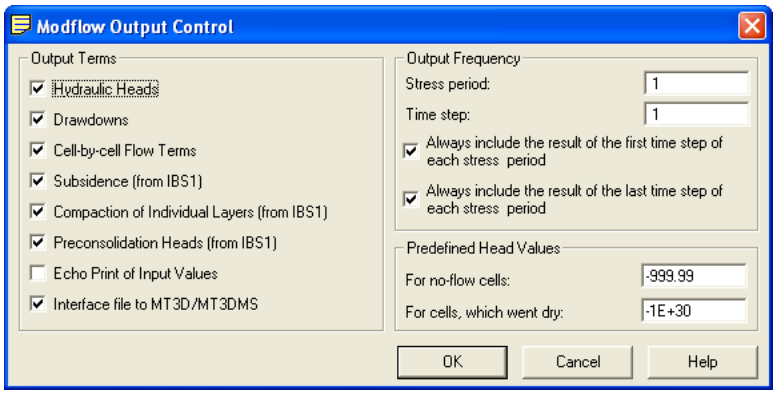


Fig. 2.36. The Modflow Output Control dialog box

  - *Drawdowns* are the differences between the initial hydraulic heads and the calculated hydraulic heads. Drawdowns in each cell are saved in the unformatted (binary) file DDOWN.DAT.
  - *Cell-by-cell Flow Terms* are flow terms for individual cells, including four types:
    1. cell-by-cell stress flows, or flows into or from an individual cell due to one of the external stresses (excitations) represented in the model, e.g., pumping well or recharge;
    2. cell-by-cell storage terms, which give the rate of accumulation or depletion of storage in an individual cell;
    3. cell-by-cell constant-head flow terms, which give the net flow to or from individual constant head cells; and
    4. internal cell-by-cell flows, which are the flows across individual cell faces, that is, between adjacent model cells. The cell-by-cell flow terms are used for calculating water budgets and for particle tracking and transport simulations by PMPATH and MOC3D. The cell-by-cell flow terms are saved in the unformatted (binary) file BUDGET.DAT.
  - *Subsidence* is the sum of the compaction of all model layers, for which the interbed storage calculation is turned on (see Section 2.4.2).
  - *Compaction of individual layers* is the sum of the calculated compaction and the user-specified starting compaction in each layer.
  - *Preconsolidation head* is the previous minimum head value in the aquifer. For model cells in which the specified preconsolidation head is greater than the corresponding value of the starting head, the preconsolidation head will be set to the starting head. Subsidence, compaction and preconsolidation head are saved in the unformatted (binary) file INTERBED.DAT.
  - *Interface file to MT3D* is an unformatted (binary) file containing the computed heads, fluxes across cell interfaces in all directions and locations and flow rates of the various sinks/sources. The interface file is created for the transport models MT3D, MT3DMS, RT3D, and PHT3D.
- *Output Frequency*: The simulation results are saved whenever the time steps and stress periods are an even multiple of the output frequency and the results for the first and last stress periods and time steps are always saved. Use 0 (zero) for the output frequency, if only the result of the last stress period or the last time step should be saved.
- *Predefined Head Values*: The predefined heads for no-flow cells (HNOFLO) and dry cells (HDRY) are given in the Predefined Head Values group.

2.6.1.19 MODFLOW | Run

Select this menu item to open the Run Modflow dialog box (Fig. 2.37) to run the flow simulation with MODFLOW or to check the model data. The available settings of the dialog box are described below.

- The File Table has three columns:

  - *Generate*: Prior to running a flow simulation, **PM** uses the user-specified data to generate input files for MODFLOW and MODPATH. An input file will be generated if it does not exist or if the corresponding *Generate* box is checked. Normally, we do not need to worry about these boxes since **PM** will take care of the settings. Note that MODPATH [94][95] and/or MODPATH-PLOT [95] cannot be started from PMWIN directly. In most cases, however, the user does not need to use these programs since PMPATH includes all their features and is far easier to use. Refer to Section 6.4 for how to run MODPATH.
  - *Description* gives the names of the packages used in the flow model.
  - *Destination File* shows the paths and names of the input files of the flow model.
- Options:
  - *Regenerate all input files*: Check this option to force **PM** to generate all input files regardless the setting of the Generate boxes. This is useful if the input files have been deleted or overwritten by other programs.
  - *Generate input files only, don't start MODFLOW*: Check this option, if the user does not want to run MODFLOW. The simulation can be started at a later time or can be started at the Command Prompt (DOS box) by executing the batch file MODFLOW.BAT.
  - *Check the model data*: If this option is checked, **PM** will check the geometry of the model and the consistency of the model data as given in Table 2.6 before creating data files. The errors (if any) are saved in the file CHECK.LIS located in the same folder as the model data.
- *OK*: Click *OK* to generate MODFLOW input files. In addition to the input files, **PM** creates a batch file MODFLOW.BAT in the model folder. When all input files

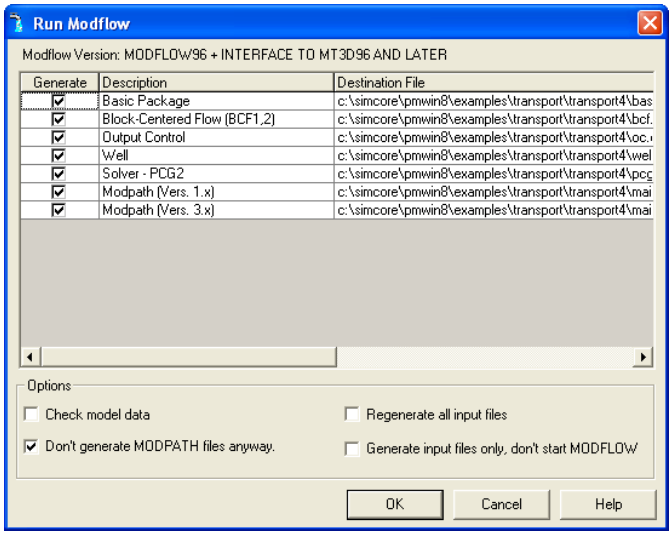


Fig. 2.37. The Run Modflow dialog box

Table 2.6 Model Data checked by **PM**

Term	**Checking Criteria**
Layer thickness	May not be zero or negative.
Top and bottom elevation of layers	Model layers may not overlap each other.
Initial head at constant head cells	A constant head cell may not be dry at the beginning of a simulation.
Horizontal hydraulic conductivity, transmissivity, vertical hydraulic conductivity, vertical leakance or effective porosity	May not be zero or negative.
Storage coefficient, specific storage, or specific yield	May not be negative.
River package	(1) A river cell may not be a fixed-head cell and should not be an inactive cell. (2) Elevation of the riverbed should be higher than the elevation of the cell bottom. (3) The river stage must be higher than elevation of the riverbed.
Streamflow-Routing package	A STR-cell may not be a constant head cell and should not be an inactive cell.
Drain package	(1) A drain cell may not be a fixed-head cell and should not be an inactive cell. (2) Elevation of the drain should be higher than the elevation of the cell bottom.
General head boundary	A GHB-cell may not be a fixed-head cell and should not be an inactive cell.
Well package	A well-cell may not be a fixed-head cell and should not be an inactive cell.

are generated, **PM** automatically runs MODFLOW.BAT in a Command Prompt-window (DOS box). During a flow simulation, MODFLOW writes a detailed run record to the file OUTPUT.DAT saved in the model folder. MODFLOW saves the simulation results in various unformatted (binary) files only if a flow simulation has been successfully completed. See *MODFLOW | Output Control* (page 74) for details about the output terms of MODFLOW.

2.6.1.20 MODFLOW | View

MODFLOW | View | Run Listing File

Select this menu item to use the Text Viewer (see Section 2.3.4) to display the run list file OUTPUT.DAT, which contains a detailed run record saved by MODFLOW.

MODFLOW | View | Head Scatter Diagram

This menu item is available only if Head Observations have been defined (see Section 2.6.1.14). Select this menu item to open the Scatter Diagram (Hydraulic Head) dialog box (Fig. 2.38). The options are grouped under two tabs – *Data* and *Chart* – as described below.

- The *Data Tab* contains a table showing the observed and calculated values at active observation boreholes (see Section 2.6.1.14 for the definition of observation boreholes). The columns of this table are listed:
  - *Plot*: A borehole will be displayed on the scatter diagram only when its Plot box is checked.
  - *Color*: Defines the plot color for each borehole. Click the button to change the color.
  - *OBSNAM*: Displays the name of each observation borehole specified in the Head Observation dialog box (Section 2.6.1.14).
  - *Calculated value*: Displays simulated head values at observation boreholes. If a borehole lies in an inactive or dry cell, the default value for dry cells

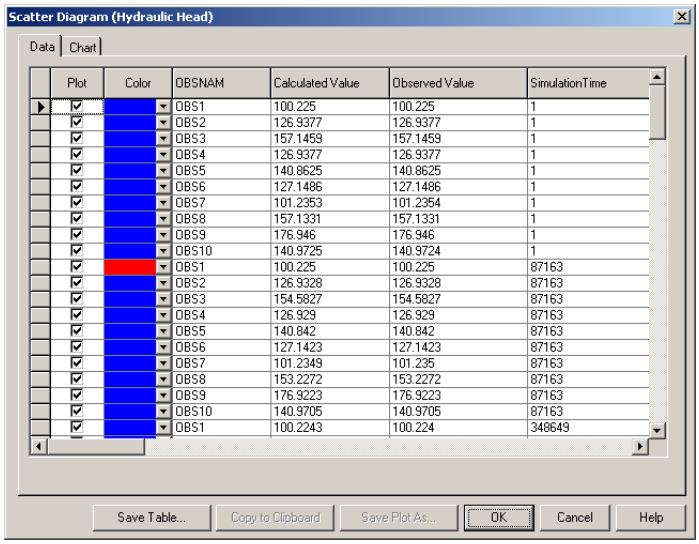


Fig. 2.38. The Data tab of the Scatter Diagram (Hydraulic Head) dialog box

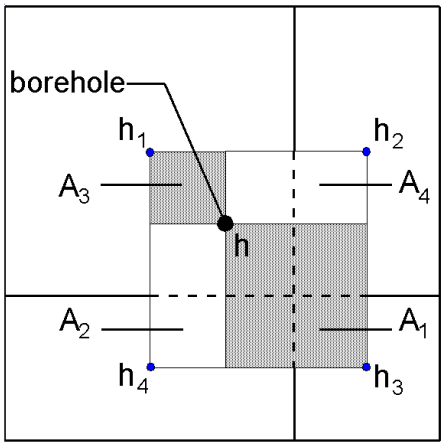


Fig. 2.39. Interpolation of simulated head values to an observation borehole

(defined in *Models* | *MODFLOW* | *Output Control*) is displayed. As observation boreholes are rarely located at cell centers, simulated head values at observation boreholes need to be calculated by means of interpolation.
At an observation borehole screened in the i-th layer (single-layer observation), **PM** calculates the simulated hydraulic head value H_i by interpolating within the layer using the following equation:

$$H_i = \frac{\sum_{j=1}^{4} (h_j \cdot A_j)}{\sum_{j=1}^{4} A_j} \qquad A_j = 0 \text{ for inactive cells} \tag{2.34}$$

where A_j are the areas and h_j are the computed values at the center of the cells surrounding the observation borehole (Fig. 2.39). For a multi-layer observation borehole, the simulated head value is calculated by equation 2.33 (page 72) using the H_i values of all screened layers.

- *Observed Value*: The user-specified observed values in the Head Observations dialog box (Section 2.6.1.14) are linearly interpolated to the simulation times and displayed in this column.
- *Simulation Time*: Displays the times at the end of each stress period or time step, to which the calculated values and observed values pertain.
- *Save Table*: Press this button to save the data of OBSNAM, Calculated Value, Observed Value and Simulation Time in an ASCII file. This button is enabled only when the Data tab is chosen.

- The *Chart Tab* (Fig. 2.40) displays the scatter diagram using the calculated and observed data. Scatter diagrams are often used to present the quality of calibration results. The observed values are plotted on one axis against the corresponding calculated values on the other. If there is an exact agreement between

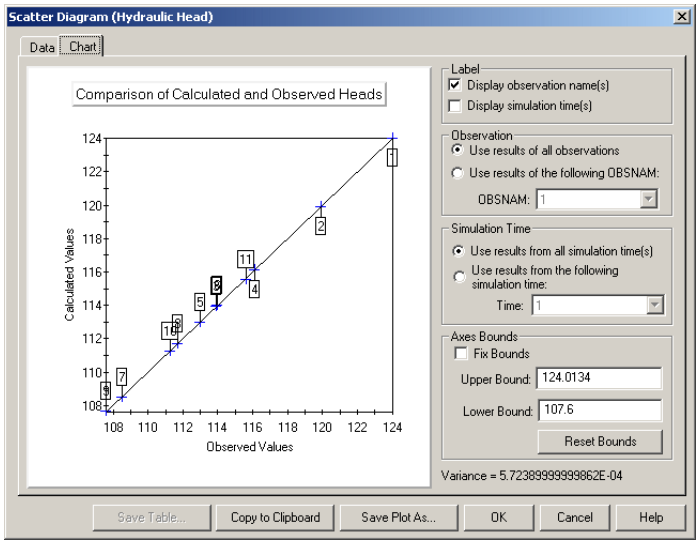


Fig. 2.40. The Chart tab of the Scatter Diagram (Hydraulic Head) dialog box

measurement and simulation, all points lie on a 45° line. The narrower the area of scatter around this line, the better is the match. The available settings are summarized below.

- Scatter Diagram: The Scatter Diagram has a lot of built-in features:
  * Right-click on the scatter diagram to open a 2D-Chart Control Properties dialog box, which allows the user to change the titles and axes settings. Most options of this dialog box are self-explanatory, however, the user can click the *Help* button for detailed descriptions of all options.
  * To zoom an area of the scatter diagram: Press the *Shift* or the *Ctrl* key, and hold down left mouse button. Drag mouse to select zoom area and release the mouse button. Performing a zoom with the *Ctrl* key enlarges the selected area of a chart, while not necessarily showing the axes.
  * To remove the zooming effect, press the ”r” key.
- *Label*: Check the boxes to display the name of the observation boreholes or the observation times on the scatter diagram.
- *Observation*: Select Use results of all observations if all Plot-marked observations listed in the *Data* table should be used. If the option Use results of the following OBSNAM is chosen, only the results of the selected observation borehole (OBSNAM) are displayed.
- *Simulation Time*: Select Use results of all simulation time(s) if all results listed in the Data table should be used. If the option Use results of the following simulation time is chosen, only the results of the selected simulation time are displayed.
- *Axes Bounds*: The bounds of the axes are defined by *Upper Bound* and *Lower Bound*, which are determined automatically if the *Fix Bounds* box is not

checked or if the *Reset Bounds* button is pressed. When editing the upper and lower bounds the scatter diagram will be updated accordantly if *Fix Bounds* is not checked. Check it to fix the bounds at specified values.
- *Variance* is the mean squared error between observed and calculated value of Plot-marked observations, which are displayed on the scatter diagram.
- *Copy to Clipboard*: Press this button to place a copy of the scatter diagram on the clipboard. The user can recall this copy by pressing Ctrl+v in almost all word or graphics processing software. This button is enabled only when the Chart tab is chosen.
- *Save Plot As*: Press this button to save the scatter diagram in Windows bitmap or Metafile formats. This button is enabled only when the Chart tab is chosen.

MODFLOW | View | Drawdown Scatter Diagram

This menu item is available only if Drawdown Observations have been defined (see Section 2.6.1.15). Select this menu item to open a Scatter Diagram (Drawdown) dialog box, which is identical to the Scatter Diagram (Hydraulic Head) dialog box (Fig. 2.38), except the drawdown values replace the head values. Note that drawdown is defined by $h_0 - h$, where h_0 is the user-specified initial hydraulic head and h is the calculated head at time t.

MODFLOW | View | Subsidence Scatter Diagram

This menu item is available only if Subsidence Observations have been defined (see Section 2.6.1.16). Select this menu item to open a Scatter Diagram (Subsidence) dialog box, which is identical to the Scatter Diagram (Hydraulic Head) dialog box (Fig. 2.38), except the subsidence values replace the head values.

MODFLOW | View | Compaction Scatter Diagram

This menu item is available only if Compaction Observations have been defined (see Section 2.6.1.17). Select this menu item to open a Scatter Diagram (Compaction) dialog box, which is identical to the Scatter Diagram (Hydraulic Head) dialog box (Fig. 2.38), except the compaction values replace the head values.

MODFLOW | View | Head-Time Curves

This menu item is available only if Head Observations have been defined (see Section 2.6.1.14). Select this menu item to open the Time Series Curves (Hydraulic Head) dialog box (Fig. 2.41). The options are grouped under two tabs: *Data* and *Chart* as described below.

- The Data Tab The Data tab contains two tables. The table to the left shows the names (OBSNAM) of the observation boreholes and their Plot and Color set-

tings. The table to the right shows the Observation Time, Calculated Values and Observed Values.

- *OBSNAM*: This column displays the name of each observation borehole specified in the Head Observation dialog box (Fig. 2.35).
- *Plot*: The time-series curves of a borehole will be displayed only when its Plot box is checked.
- *Color*: This column defines the plot color for each borehole. Click the button to change the color.
- *Simulation Time*: Displays the times at the end of each stress period or time step, to which the calculated values and observed values pertain.
- *Calculated value*: Displays simulated head values at observation boreholes. If a borehole lies in an inactive or dry cell, the default value for dry cells (defined in *Models* | *MODFLOW* | *Output Control*) is displayed. Refer to *MODFLOW* | *View* | *Head Scatter Diagram* (page 78) for details of interpolating simulated heads to the observation boreholes.
- *Observed Value*: The user-specified observed values in the Head Observations dialog box (Fig. 2.35) are linearly interpolated to the simulation times and displayed in this column.
- Save Table: Press this button to save the data of OBSNAM, Simulation Time, Calculated Value, Observed Value in an ASCII file. This button is enabled only when the Data tab is chosen.

• The Chart Tab The Chart tab (Fig. 2.42) displays time-series curves using the calculated and observed values. The available settings are summarized below.

- Chart: The Chart has a lot of built-in features:

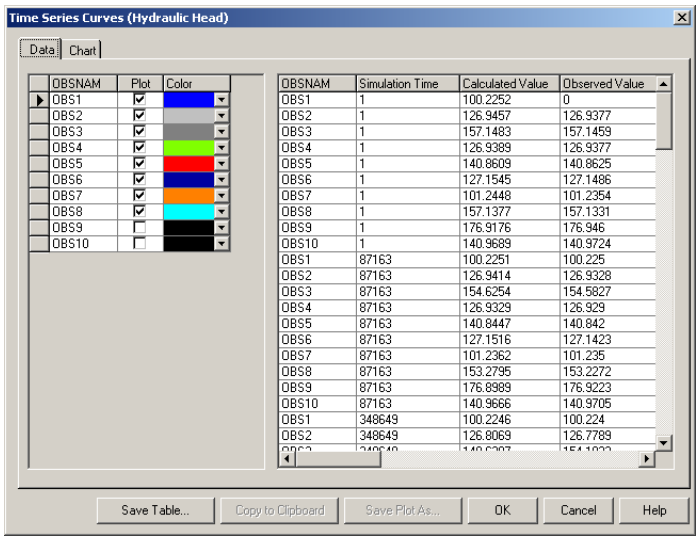


Fig. 2.41. The Data tab of the Time Series Curves (Hydraulic Head) dialog box

  * Right-click on the chart to open a 2D-Chart Control Properties dialog box, which allows the user to change the titles and axes settings. Most options of this dialog box are self-explanatory, however, the user can click the Help button for detailed descriptions of all options.
  * To zoom an area of the scatter diagram: Press the *Shift* or the *Ctrl* key, and hold down left mouse button. Drag mouse to select a zoom area and release the mouse button. Performing a zoom with the *Ctrl* key enlarges the selected area of a chart, while not necessarily showing the axes.
  * To remove the zooming effect, press the ”r” key.

– *X-Axis (Time)*: The bounds of the time axis are defined by *Upper Bound* and *Lower Bound*, which are determined automatically if the check box *Fix Bounds* is clear or if the *Reset Bounds* button is pressed. When editing the upper and lower bounds the chart will be updated accordantly if *Fix Bounds* is not checked. Check it to fix the bounds at specified values. Check *Logarithmic* to display the time-axis in the logarithmic scale.
– *Y-Axis*: The bounds of this axis are defined by Upper Bound and Lower Bound, which are determined automatically if the check box *Fix Bounds* is clear or if the Reset Bounds button is pressed. When editing the upper and lower bounds the chart will be updated accordantly if *Fix Bounds* is not checked. Check it to fix the bounds at specified values. Check *Logarithmic* to display the Y-axis in the logarithmic scale.
– *Data Type*: Check the *Calculated* or *Observed* box to display the time-series curves based on the calculated or observed values, respectively. The chart uses solid lines for displaying calculated curves. Observation curves are dashed. Select Use results of all observations if all Plot-marked observations

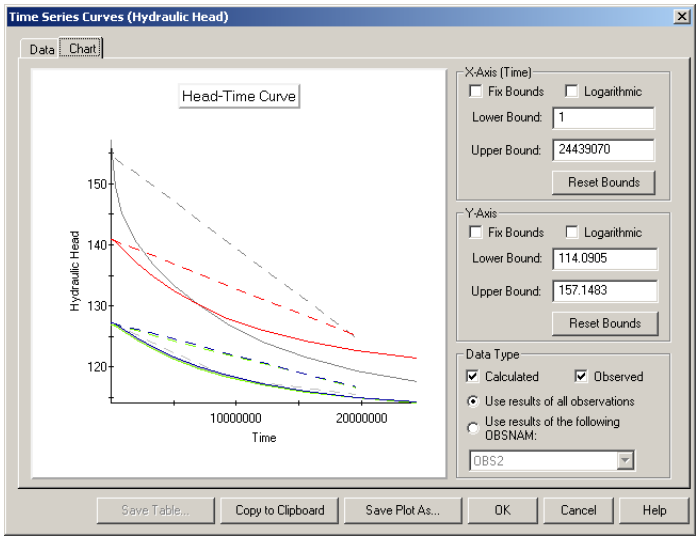


Fig. 2.42. The Chart tab of the Head-Time Series Curves Diagram dialog box

listed in the Data table should be used. If the option *Use results of the following OBSNAM* is chosen, only the curves of the selected observation borehole (OBSNAM) are displayed.

– *Copy to Clipboard*: Press this button to place a copy of the chart on the clipboard. The user can recall this copy by pressing Ctrl+v in almost all word or graphics processing software. This button is enabled only when the Chart tab is chosen.
– *Save Plot As*: Press this button to save the chart in Windows bitmap or Metafile formats. This button is enabled only when the Chart tab is chosen.

2.6.2 MT3DMS/SEAWAT

The first step to use MT3DMS or SEAWAT is to define the simulation mode, species and type of reactions to be simulated in the Simulation Settings dialog box (Section 2.6.2.1). Once the simulation settings are defined, the appropriate menu items of the MT3DMS/SEAWAT menu will be enabled allowing the user to specify required model parameters. If the user selects menu items involving species-dependent parameters, **PM** will display a dialog box for selecting a species, for which the parameter is to be specified. For example, if you select *MT3DMS/SEAWAT | Initial Concentration*, the Initial Concentration dialog box (Fig. 2.43) will appear and the following options are available.

- Select a species and click the Edit button to specify the initial concentration for that species.
- Click the Close button to close the dialog box and to stop editing data.
- The Data box has three types of status as given below. Once the data is specified, you may click on the Data box to check or clear it.
  – ☒: Data has been specified and will be used for simulation.

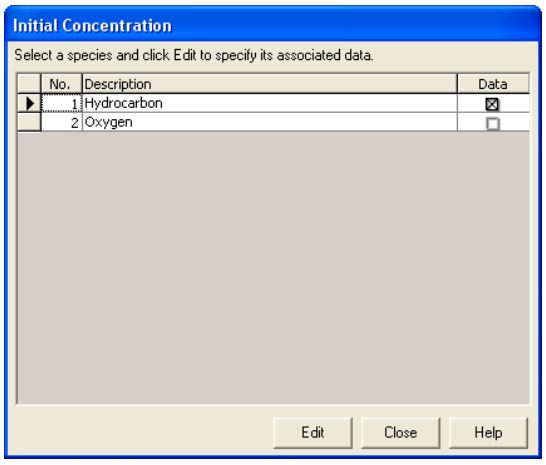


Fig. 2.43. The Initial Concentration dialog box

- ☐: Data has been specified, but will not be used; the default value of zero will be used.
- ☐: Data is not available (the box is dimmed and deactivated); the default value of zero will be used.

2.6.2.1 MT3DMS/SEAWAT | Simulation Settings

The Simulation Settings dialog box (Fig. 2.44) controls the type of reaction and the species involved in the simulation. It also controls whether variable density flow and/or transport should be simulated. The available settings are described as follows.

- *Simulation Mode*:
  - *Constant Density Transport with MT3DMS*: If this option is selected, the constant density flow solution of MODFLOW will be used by MT3DMS to simulate solute transport processes. It is assumed that the solution concentration does not affect the fluid density and the flow field. MT3DMS simulations are carried out on the basis of flow-fields computed beforehand by MODFLOW.
  - *Variable Density Flow and Transport with SEAWAT*: If this option is selected, SEAWAT will be used to simulate coupled variable-density flow and solute transport. With this option, fluid density is calculated by using an equation of state and the simulated solute concentration values of involved species. The

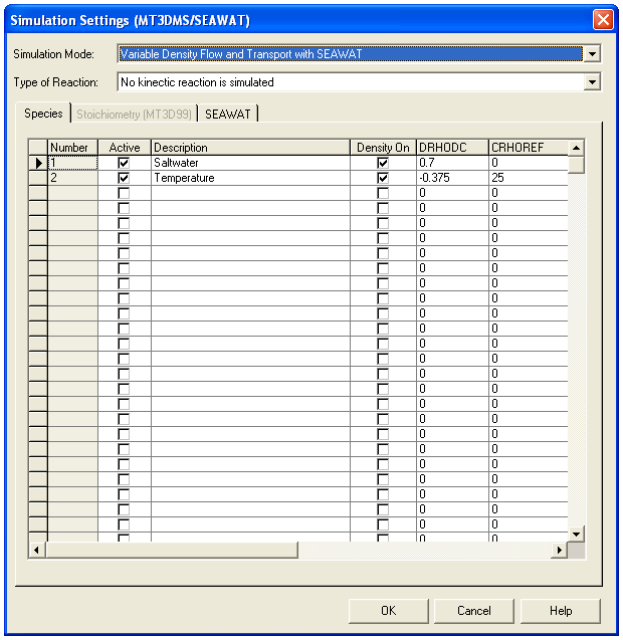


Fig. 2.44. The Simulation Settings (MT3DMS/SEAWAT) dialog box

density-effect of a particular species may be turned on or off in the Species tab (see below). The flow and transport processes are computed by MODFLOW and MT3DMS that are incorporated in SEAWAT.

- *Type of Reaction*: Select a type of reaction that you want to simulate from this dropdown box. MT3DMS includes the type of *First-order irreversible reaction* only. The last three reaction types are supported by the proprietary MT3D99 code [122]. If you do not have access to MT3D99 or need to simulate more complex reaction scenarios, consider using the multicomponent reactive transport model PHT3D, see Section 2.6.3 for details.
  The required parameters for the selected chemical reaction type are specified by selecting *MT3DMS/SEAWAT | Chemical Reaction* (see Section 2.6.2.6).
  - *No kinetic reaction is simulated*: Select this one to turn off the simulation of kinetic reactions.
  - *First-order irreversible reaction* simulates radioactive decay or biodegradation.
  - *Monod kinetics* MT3D99 implements the Monod kinetics only for the dissolved phase of an organic compound.
  - *First-order parent-daughter chain reactions* can be used to model radioactive chain reaction and biodegradation of chlorinated solvents, for example the transformation of perchloroethene (PCE) → trichloroethene (TCE)→ dichloroethene (DCE) → vinyl chloride (VC). The species are defined in the Species tab and the yield coefficients between species pairs are to be specified in the Stoichiometry tab of the Simulation Settings dialog box (Fig. 2.45).
  - *Instantaneous reaction among species*: MT3D99 uses the approach of Borden and Bedient [15] and Rifai and others [102][103] to simulate the aerobic and anaerobic biodegradation of common hydrocarbon contaminants, including benzene, touluene, ethylbenzene, and xylene (BTEX). Stoichiometric ratios between the first species and other species are required to simulate this type of reaction and are to be specified in the Stoichiometry tab (Fig. 2.45).
- *Species tab* (Fig. 2.44). The columns of the table are described below:
  - *Number*: This column displays the (read-only) species number.
  - *Active*: Check the Active box to add a species to the simulation.
  - *Description*: Type the name or description of the species here.
  - *Density On*: This item is used by SEAWAT only. Check the box to include the concentration of the simulated species in the fluid density calculation. If the fluid density is independent of all simulated species (i.e., *Density On* boxes of all species are cleared), SEAWAT will run in a *uncoupled mode* and the user-specified fluid density array (see Section 2.6.2.7) will be used in the simulation.
  - *DRHODC*: This item is used by SEAWAT only. DRHODC (i.e., $\partial\rho/\partial C$) is the slope that relates fluid density (ρ) to solute concentration (C). Separate values for DRHODC are entered for individual species. DRHODC is ignored if the *Density On* box of the corresponding species is not checked. Any mea-

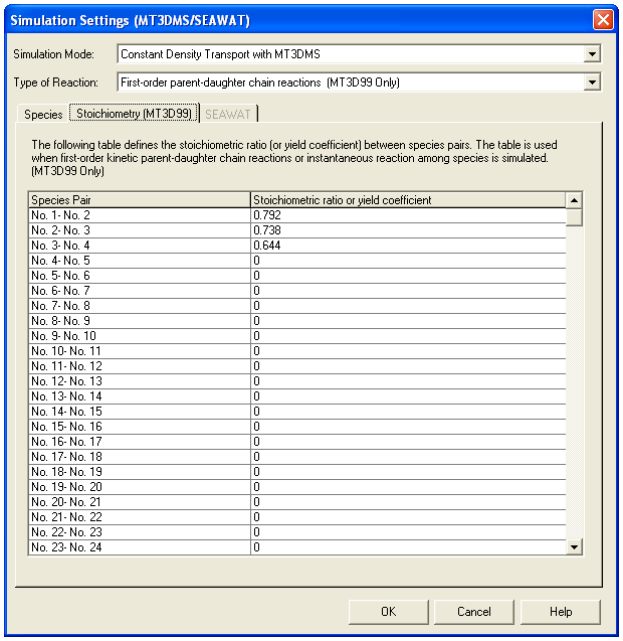

Simulation Settings (MT3DMS/SEAWAT)
Simulation Mode:
Constant Density Transport with MT3DMS
Type of Reaction:
First-order parent-daughter chain reactions (MT3D99 Only)
Species
Stoichiometry (MT3D99)
SEAWAT
The following table defines the stoichiometric ratio (or yield coefficient) between species pairs. The table is used when first-order kinetic parent-daughter chain reactions or instantaneous reaction among species is simulated. (MT3D99 Only)
Species Pair
Stoichiometric ratio or yield coefficient
No. 1- No. 2 0.792
No. 2- No. 3 0.738
No. 3- No. 4 0.644
No. 4- No. 5 0
No. 5- No. 6 0
No. 6- No. 7 0
No. 7- No. 8 0
No. 8- No. 9 0
No. 9- No. 10 0
No. 10- No. 11 0
No. 11- No. 12 0
No. 12- No. 13 0
No. 13- No. 14 0
No. 14- No. 15 0
No. 15- No. 16 0
No. 16- No. 17 0
No. 17- No. 18 0
No. 18- No. 19 0
No. 19- No. 20 0
No. 20- No. 21 0
No. 21- No. 22 0
No. 22- No. 23 0
No. 23- No. 24 0
OK
Cancel
Help

Fig. 2.45. The Stoichiometry tab of the Simulation Settings (MT3DMS/SEAWAT) dialog box

surement unit can be used for solute concentration, provided DRHODC and the reference fluid density (DENSEREF, see below) are set properly.

– *CRHOREF*: This item is used by SEAWAT only. CRHOREF is the reference concentration for the species. For most simulations, CRHOREF should be specified as zero.

- *Stoichiometry tab* (Fig. 2.45) is used to specify yield coefficients or stoichiometric ratios between species pairs. A *yield coefficient* $Y_{1/2}$ between two species means consuming of one mass unit of species 1 will yield $Y_{1/2}$ mass units of species 2. For example, if $Y_{1/2}$ = 3 then consuming of 1 g of species 1 will yield 3 g of species 2. The *stoichiometric ratio* F_{1k} between species 1 and species k means one mass unit of species 1 reacts with F1k mass units of species k. For example, if F_{14} = 3 then 1 g of species 1 will react with 3 g of species 4.
- *SEAWAT tab* (Fig. 2.46) is used to specify SEAWAT simulation control parameters. The available settings are given below.
  – *Activate the variable-density water-table correction (IWTABLE)*: Check this option to activate the variable-density water-table corrections (eq. 82 of [51]).
  – *Method for calculating internodal density values*: This option determines how the internodal density values used to conserve fluid mass will be calculated.
  – *Flow and transport coupling procedure*:

    * *One-Timestep lag*: Flow and transport will be explicitly coupled using a *one timestep lag* as described in Guo and Langevin [51]. With the explicit approach, the flow equation is formulated using fluid densities from the previous transport timestep. The explicit coupling option is normally much faster than the iterative option and is recommended by the authors of SEAWAT [77] for most applications.
    * *Non-linear Iterative*: The solution of the flow and transport equations is obtained in an iterative sequence for each timestep until the consecutive differences in the calculated fluid densities are less than a user-specified value. See Guo and Langevin [51] for detailed explanations.
    * *Conditional*: The flow solution will be recalculated only for: (1) The first transport step of the simulation, or (2) The last transport step of the MODFLOW timestep, or (3) The maximum density change at a cell is greater than the *Density change threshold for recalculating flow solution* (see below).
- *Maximum number of non-linear coupling iterations*: This value is used only if the *Flow and transport coupling procedure* is *Non-linear Iterative*. SEAWAT will stop execution after the given number iterations for the flow and transport solutions if convergence has not occurred.
- *Density change convergence criterion for coupling iterations [M/L^3]*: This value is used only if the *Flow and transport coupling procedure* is *Non-linear Iterative*. If the maximum fluid density difference between two consecutive implicit coupling iterations is less than then given value, SEAWAT will advance to the next timestep. Otherwise, SEAWAT will continue to iterate on the flow and transport equations, or will terminate if *Maximum number of non-linear coupling iterations* is reached.
- *Density change threshold for recalculating flow solution [M/L^3]*: This value is used only if the *Flow and transport coupling procedure* is *Conditional*. If the fluid density change (between the present transport timestep and the last flow solution) at one or more cells is greater than the given value, then SEAWAT will update the flow field (by solving the flow equation with the updated density field).
- *Length of the first transport time step (FIRSTDT)*: This is the length of the first transport timestep used to start the simulation.
- *Reference fluid density (DENSEREF)*: DENSEREF is the fluid density at the reference concentration, temperature, and pressure. For most simulations, DENSEREF is specified as the density of freshwater at 25 C and at a reference pressure of zero.
- *Minimum Fluid Density (DENSEMIN)*: .
    * If DENSEMIN > 0: If the computed fluid density is less than DENSEMIN, the density value is set to DENSEMIN.
    * If DENSEMIN $= 0$: The computed fluid density is not limited by DENSEMIN.
- *Maximum Fluid Density (DENSEMAX)*:
    * If DENSEMAX > 0, If the computed fluid density is greater than DENSEMAX, the density value is set to DENSEMAX.

  * If DENSEMAX = 0, The computed fluid density is not limited by DENSEMAX.
- *Density Options - uncoupled mode*: When the all *Density On* boxes in the Species tab are cleared (i.e., SEAWAT runs in a *uncoupled mode*), the user has the option to determine the density of the source fluid at wells, river and general-head boundaries. If *Reference Fluid Density* is selected, then density value of the source fluid is equal to DENSEREF, otherwise the user-specified density values to the respective packages will be used.

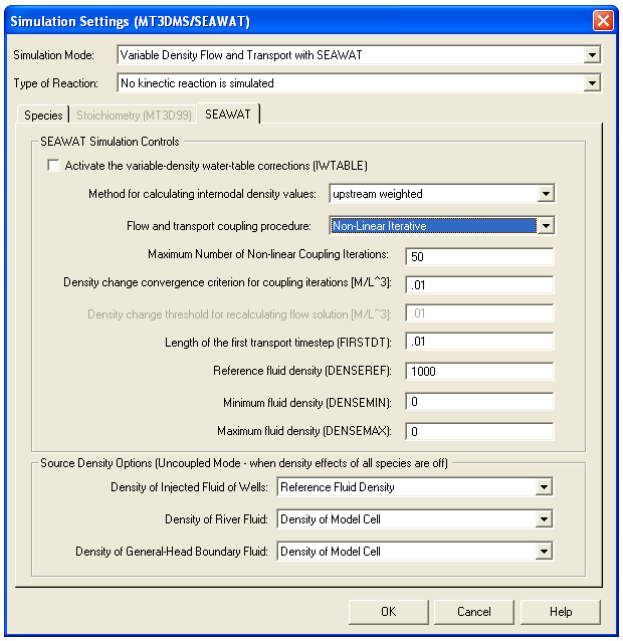


Fig. 2.46. The Variable Density tab of the Simulation Settings (MT3DMS/SEAWAT) dialog box

2.6.2.2 MT3DMS/SEAWAT | Initial Concentration

At the beginning of a transport simulation, MT3DMS and SEAWAT require the initial concentration of each active species at each active concentration cell, i.e. ICBUND > 0.

2.6.2.3 MT3DMS/SEAWAT | Advection

The available settings of the Advection Package (MT3DMS) dialog box (Fig. 2.47) are described below.

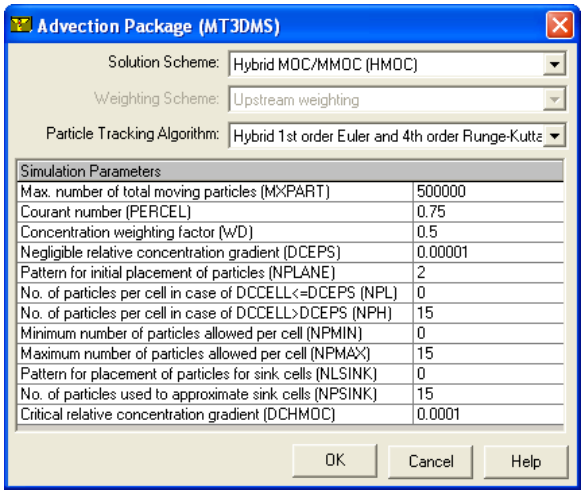

Advection Package (MT3DMS)
Solution Scheme: Hybrid MOC/MMOC (HMOC)
Weighting Scheme: Upstream weighting
Particle Tracking Algorithm: Hybrid 1st order Euler and 4th order Runge-Kutta
Simulation Parameters
Max. number of total moving particles (MXPART) 500000
Courant number (PERCEL) 0.75
Concentration weighting factor (WD) 0.5
Negligible relative concentration gradient (DCEPS) 0.00001
Pattern for initial placement of particles (NPLANE) 2
No. of particles per cell in case of DCCELL<=DCEPS (NPL) 0
No. of particles per cell in case of DCCELL>DCEPS (NPH) 15
Minimum number of particles allowed per cell (NPMIN) 0
Maximum number of particles allowed per cell (NPMAX) 15
Pattern for placement of particles for sink cells (NLSINK) 0
No. of particles used to approximate sink cells (NPSINK) 15
Critical relative concentration gradient (DCHMOC) 0.0001
OK
Cancel
Help

Fig. 2.47. The Advection Package (MT3DMS) dialog box

- *Solution Scheme*: MT3DMS provides five solution schemes for the advection term, as described below.
  - The *method of characteristics (MOC)* scheme was implemented in the transport models MOC [73] and MOC3D (see Section 2.6.5.3), and has been widely used. One of the most desirable features of the MOC technique is that it is virtually free of numerical dispersion, which creates serious difficulty in many numerical schemes. The major drawback of the MOC scheme is that it can be slow and requires a large amount of computer memory when a large number of particles is required. Also, the computed concentrations sometimes tend to show artificial oscillations.
  - The *modified method of characteristics (MMOC)* uses one particle for each finite-difference cell and is normally faster than the MOC technique. At each new time level, a particle is placed at the nodal point of each finite-difference cell. The particle is tracked backward to find its position at the old time level. The concentration associated with that position is used to approximate the advection-relevant average concentration at the cell, where the particle is placed. The MMOC technique is free of artificial oscillations if implemented with a lower-order velocity interpolation scheme (such as linear interpolation used in MT3D and MT3DMS). However, with a lower-order velocity interpolation scheme, the MMOC technique introduces some numerical dispersion, especially for sharp front problems.
  - The *hybrid method of characteristics (HMOC)* attempts to combine the strengths of the MOC and MMOC schemes by using an automatic adaptive scheme conceptually similar to the one proposed by Neumann [89]. The fundamental idea behind the scheme is automatic adaptation of the solution process to the nature of the concentration field. When sharp concentration fronts are present, the advection term is solved by MOC through the use of

moving particles dynamically distributed around each front. Away from such fronts, the advection term is solved by MMOC. The criterion for controlling the switch between the MOC and MMOC schemes is given by DCHMOC (see below).

- The *finite-difference method* is implicit with the Generalized Conjugate Gradient solver (GCG) package (see Section 2.6.2.10).
  Due to the problems of numerical dispersion and artificial oscillation, the upstream finite difference method is only suitable for solving transport problems not dominated by advection. When the grid Peclet number P_e ($P_e = \Delta x/\alpha L$; Δx is the grid spacing and αL is the longitudinal dispersivity) is smaller than two, the upstream finite difference method is reasonably accurate. However, it is advisable to use the upstream finite difference method for obtaining first approximations in the initial stages of a modeling study.
- The *third-order TVD method* is based on the ULTIMATE algorithm [80] [81][82], which is in turn derived from the earlier QUICKEST algorithm [79]. With the ULTIMATE scheme, the solution is mass conservative, without excessive numerical dispersion and artificial oscillation.

- *Weighting Scheme* is needed only when the implicit finite-difference method is used, i.e., the solution scheme is finite-difference and the iterative GCG solver is used. In the finite-difference method, when computing the mass flux into a model cell by advection, the concentration values at the cell interfaces between two neighboring cells are used. For the upstream weighting scheme, the interface concentration in a particular direction is equal to the concentration at the upstream node along the same direction. For the central-in-space weighting scheme, the interface concentration is obtained by linear interpolation of the concentrations at the two neighboring cells.
  As denoted in Zheng and Wang [121], the central-in-space scheme does not lead to intolerable numerical dispersion when the grid spacing is regular. However, if transport is dominated by advection, the upstream weighting is preferred, as the central-in-space weighting scheme can lead to excessive artificial oscillation.
- *Particle Tracking Algorithm* is used in combination with the method of characteristics.
  - Using the *first-order Euler algorithm*, numerical errors tend to be large unless small transport steps are used. The allowed transport step t of a particle is determined by MT3D using equation 2.35

$$|\Delta t| \leq \gamma_c \cdot R \cdot MIN\left[\frac{\Delta x}{v_x}, \frac{\Delta y}{v_y}, \frac{\Delta z}{v_z}\right] \tag{2.35}$$

    where Δx, Δy, and Δz are the cell widths along the row, column, and layer directions, respectively; c is the Courant number. The particle velocities v_x, v_y, and v_z at the position (x, y, z) are obtained by linear interpolation from the specific discharges at the cell faces. The minimum Δt of all particles is used in a transport step.
  - The basic idea of the *fourth-order Runge-Kutta method* is to calculate the particle velocity four times for each tracking step: one at the initial point,

twice at two trial midpoints, and once at a trial end point. A weighted velocity based on values evaluated at these four points is used to move the particle to a new position. The fourth-order Runge-Kutta method permits the use of larger tracking steps. However, its computational effort is considerably larger than the first-order Euler method. For this reason a mixed option combining both methods is introduced in MT3DMS.

  - The mixed option is implemented by automatic selection of the fourth-order Runge-Kutta algorithm for particles located in cells which contain or are adjacent to sinks or sources, and automatic selection of the first-order Euler algorithm for particles located elsewhere.

- *Simulation Parameters*: Depends on the selected *Solution Scheme*, one or more of the following parameters may be required.
  - *Maximum number of total moving particles (MXPART)* is the number of particles allowed in a simulation.
  - *Courant number (PERCEL)* is the number of cells (or a fraction of a cell) any particle will be allowed to move in any direction in one transport step. Generally, $0.5 \leq \text{PERCEL} \leq 1$.
  - *Concentration-weighting factor (WD)* lies between 0 and 1. The value of 0.5 is normally a good choice. This number can be adjusted to achieve better mass balance. Generally, it can be increased toward 1 as advection becomes more dominant.
  - *Negligible relative concentration gradient (DCEPS)* is a criterion for placing particles. A value around 10^{-5} is generally adequate. If DCEPS is greater than the relative cell concentration gradient $DCCELL_{k,i,j}$ (equation 2.36), NPH particles are placed in the cell [k, i, j], otherwise NPL particles are placed (see NPH and NPL below).

$$DCCELL_{k,i,j} = \frac{CMAX_{k,i,j} - CMIN_{k,i,j}}{CMAX - CMIN} \tag{2.36}$$

    where $CMAX_{k,i,j}$ and $CMIN_{k,i,j}$ are the maximum and minimum concentration values in the immediate vicinity of the cell [k, i, j]; CMIN and CMAX are the minimum and maximum concentration values in the entire grid, respectively.
  - *Pattern for initial placement of particles (NPLANE)* is used to select a pattern for initial placement of moving particles.
    * NPLANE = 0, the random pattern is selected for initial placement. Particles are distributed randomly in both the horizontal and vertical directions (Fig. 2.48b). This option generally leads to smaller mass balance discrepancy in nonuniform or diverging/converging flow fields.
    * NPLANE > 0, the fixed pattern is selected for initial placement. The value of NPLANE serves as the number of "planes" on which initial particles are placed within each cell (Fig. 2.48a). This fixed pattern may work better than the random pattern only in relatively uniform flow fields. For two dimensional simulations in plan view, set NPLANE=1. For cross

sectional or three dimensional simulations, NPLANE=2 is normally adequate. Increase NPLANE if more resolution in the vertical direction is desired.

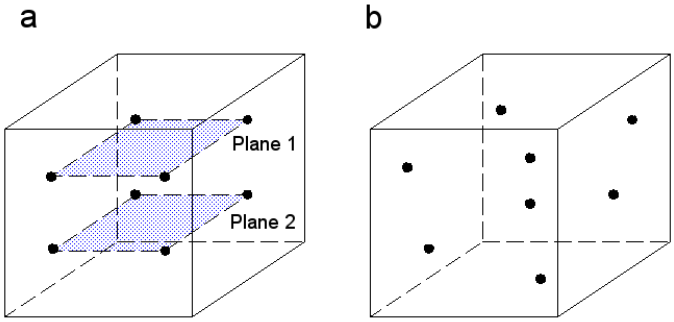


Fig. 2.48. Initial placement of moving particles (adapted from Zheng [117]): (a) Fixed pattern, 8 particles are placed on two planes within a cell. (b) Random pattern, 8 particles are placed randomly within a cell.

- *No. of particles per cell in case of DCCELL $\leq$= DCEPS (NPL)* is the number of initial particles per cell to be placed at cells where the relative cell concentration gradient DCCELL is less than or equal to DCEPS. Generally, NPL can be set to zero since advection is considered insignificant under the condition DCCELL $\leq$ DCEPS. Setting NPL equal to NPH causes a uniform number of particles to be placed in every cell over the entire grid (i.e., the uniform approach).
- *No. of particles per cell in case of DCCELL $>$ DCEPS (NPH)* is the number of initial particles per cell to be placed at cells where the relative cell concentration gradient DCCELL is greater than DCEPS. The selection of NPH depends on the nature of the flow field and also the computer memory limitation. Generally, use a smaller number in relatively uniform flow fields and a larger number in relatively nonuniform flow fields. However, values exceeding 16 in two-dimensional simulations or 32 in three dimensional simulations are rarely necessary. If the random pattern is chosen, NPH particles are randomly distributed within the cell. If the fixed pattern is chosen, NPH is divided by NPLANE to yield the number of particles to be placed per plane, which is rounded to one of the values shown in Fig. 2.49.
- *Minimum number of particles allowed per cell (NPMIN)*: If the number of particles in a cell at the end of a transport step is fewer than NPMIN, new particles are inserted into that cell to maintain a sufficient number of particles. NPMIN can be set to 0 in relatively uniform flow fields, and a number greater than zero in diverging/converging flow fields. Generally, a value between zero and four is adequate.

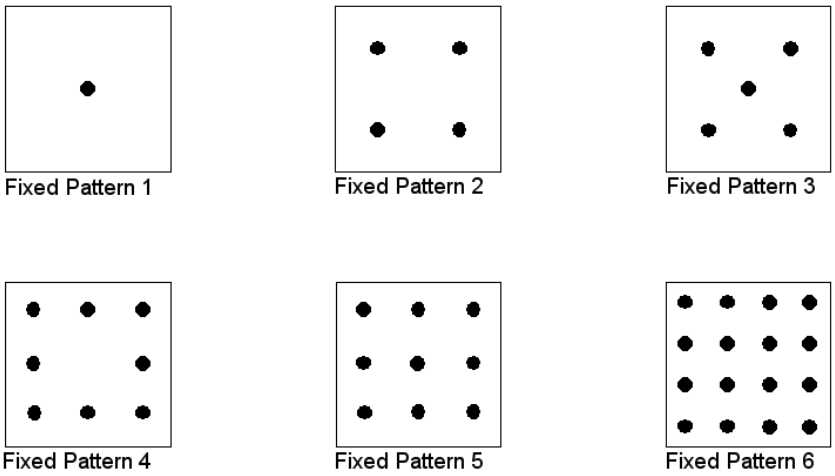
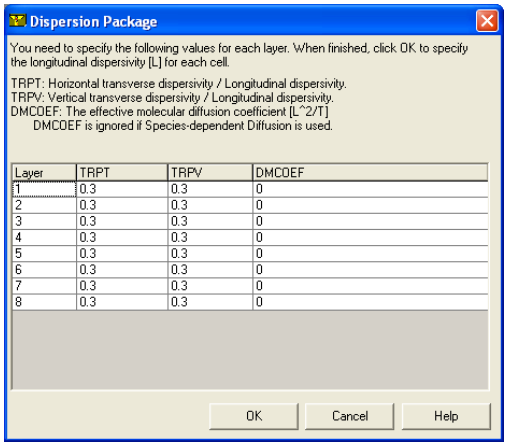


Fig. 2.49. Distribution of initial particles using the fixed pattern (adapted from Zheng 1990) If the fixed pattern is chosen, the number of particles placed per cell (NPL and NPH) is divided by the number of planes NPLANE to yield the number of particles to be placed on each plane, which is then rounded to one of the numbers of particles shown here.

- *Maximum number of particles allowed per cell (NPMAX)*: If the number of particles in a cell exceeds NPMAX, particles are removed from that cell until NPMAX is met. Generally, NPMAX $\simeq 2 \times$ NPH.
- SRMULT is a multiplier for the particle number at source cells (SRMULT $\geq$ 1). In most cases, SRMULT = 1 is sufficient. However, better results may be obtained by increasing SRMULT.
- *Pattern for placement of particles for sink cells (NLSINK)* is used to select a pattern for initial placement of particles to approximate sink cells in the MMOC scheme. The convention is the same as that for NPLANE and it is generally adequate to set NLSINK equivalent to NPLANE.
- *Number of particles allowed to approximate sink cells (NPSINK)* is used in the MMOC scheme. The convention is the same as that for NPH and it is generally adequate to set NPSINK equivalent to NPLANE.
- *Critical relative concentration gradient (DCHMOC)* is used to select between MOC and MMOC in the HMOC solution scheme. MOC is selected at cells where DCCELL $>$ DCHMOC. MMOC is selected at cells where DCCELL $\leq$ DCHMOC.

2.6.2.4 MT3DMS/SEAWAT | Dispersion

The following values must be specified for each layer in the Dispersion Package dialog box (Fig. 2.50).


Dispersion Package
You need to specify the following values for each layer. When finished, click OK to specify the longitudinal dispersivity [L] for each cell.
TRPT: Horizontal transverse dispersivity / Longitudinal dispersivity.
TRPV: Vertical transverse dispersivity / Longitudinal dispersivity.
DMCOEF: The effective molecular diffusion coefficient [L^2/T]
DMCOEF is ignored if Species-dependent Diffusion is used.
Layer TRPT TRPV DMCOEF
1 0.3 0.3 0
2 0.3 0.3 0
3 0.3 0.3 0
4 0.3 0.3 0
5 0.3 0.3 0
6 0.3 0.3 0
7 0.3 0.3 0
8 0.3 0.3 0
OK
Cancel
Help
Fig. 2.50. The Dispersion Package dialog box

- *TRPT* is the ratio of the horizontal transverse dispersivity to the longitudinal dispersivity. The longitudinal dispersivity for each finite-difference cell is specified in the Data Editor. *Longitudinal dispersivity* is used to approximate the spreading of the solute concentration in groundwater caused by the irregular shape of the interconnected pore space and the velocity variations at the microscopic level as well as the unresolved macroscopic level. The velocity of groundwater varies according to the size of the pores and water moves faster at the internal points between soil grains than on the solid surface. This spreading is often referred to as mechanical dispersion and it occurs in all three spatial directions. The coefficient of mechanical dispersion is defined by $\alpha_i \cdot v_i$, where α_i is the dispersivity and v_i is the average linear velocity in the i-direction. The sum of mechanical dispersion and molecular diffusion is called hydrodynamic dispersion.
  Values of dispersivity used for simulations generally depend on the scale of a concentration plume being considered. While a plume ”grows”, it will not only undergo the microscopic mechanical dispersion but also the dispersion caused by macroscopic heterogeneities. This results in a trend of increasing dispersivity values with the scale of observation. Summaries of the scale-dependent dispersivity values can be found in Anderson [6][7], Gelhar et al. [49][50], and Spitz and Moreno [109]. Note that all heterogeneity, which is not explicitly represented in the model, should be incorporated into the dispersion coefficients.
- *TRPV* is the ratio of the vertical transverse dispersivity to the longitudinal dispersivity.
- *DMCOEF* is the effective molecular diffusion coefficient D* [L^2T^{-1}] (equation 2.38).
  DMCOEF describes the diffusive flux of a solute in water from an area of greater concentration toward an area where it is less concentrated. The mass flux is proportional to the concentration gradient and is given by Fick’s first law:

$$\overrightarrow{F} = -D \cdot \nabla C \tag{2.37}$$

where $\overrightarrow{F}$ $[ML^{-2}T^{-1}]$ is the mass flux of solute per unit area per unit time; D $[L^2T^{-1}]$ is the diffusion coefficient; C $[ML^{-3}]$ is the solute concentration and ∇C $[ML^{-3}L^{-1}]$ is the concentration gradient. In porous media, the solute mass cannot diffuse as fast as in free water, because the ions must move along longer pathways through the pore space. To account for this tortuosity effect, an effective diffusion coefficient D^* must be used.

$$D^* = \omega \cdot D \tag{2.38}$$

According to Freeze and Cherry [46], ω ranges from 0.5 to 0.01 for laboratory studies of diffusion of non-adsorbed ions in porous geologic materials. The diffusion coefficients D of the major ions (Na^+, K^+, Mg^{2+}, Ca^{2+}, Cl^-, CO_3^{2-}, HCO_3^-, SO_4^{2-}) are temperature-dependent and range from 1×10^{-9} to $2 \times 10^{-9} m^2/s$ at 25°C [83] [104]. At 5°C the coefficients are about 50% smaller. The molecular diffusion coefficient is generally very small and negligible compared to the mechanical dispersion (see below) and is only important when groundwater velocity is very low.

In MT3DMS, the concentration change due to dispersion alone is solved with a fully explicit central finite-difference scheme. There is a certain stability criterion associated with this scheme. To retain stability, the transport step size cannot exceed an upper limit defined by equation 2.39.

$$\Delta t \leq \frac{0.5 \cdot R}{\frac{D_{xx}}{\Delta x^2} + \frac{D_{yy}}{\Delta y^2} + \frac{D_{zz}}{\Delta z^2}} \tag{2.39}$$

where Δx, Δy and Δz are the widths of the cell along the row, column, and layer directions; R is the retardation factor. The components of the hydrodynamic dispersion coefficient D_{xx}, D_{yy}, and D_{zz} are calculated by equation 2.40.

$$\begin{aligned} D_{xx} &= \alpha_L \cdot \frac{v_x^2}{|v|} + \alpha_{TH} \cdot \frac{v_y^2}{|v|} + \alpha_{TV} \cdot \frac{v_z^2}{|v|} + D^* \\ D_{yy} &= \alpha_L \cdot \frac{v_y^2}{|v|} + \alpha_{TH} \cdot \frac{v_x^2}{|v|} + \alpha_{TV} \cdot \frac{v_z^2}{|v|} + D^* \\ D_{zz} &= \alpha_L \cdot \frac{v_z^2}{|v|} + \alpha_{TH} \cdot \frac{v_x^2}{|v|} + \alpha_{TV} \cdot \frac{v_y^2}{|v|} + D^* \end{aligned} \tag{2.40}$$

where α_L $[L]$ is the longitudinal dispersivity; α_{TH} $[L]$ is the horizontal transverse dispersivity; α_{TV} $[L]$ is the vertical transverse dispersivity; v_x, v_y, and v_z $[LT^{-1}]$ are components of the flow velocity vector along the x, y, and z axes; and

$$|v| = (v_x^2 + v_y^2 + v_z^2)^{1/2} \tag{2.41}$$

Equation 2.39 is calculated for each active cell and the minimum Δt is taken as the maximum allowed step size for solving the dispersion term. This criterion is compared with other transport step size constraints to determine the minimum step size for the simulation. Generally, a higher flow velocity, for example the velocity in the immediate vicinity of a pumping well, will cause larger values of D_{xx}, D_{yy}, and D_{zz}, which, in turn, result in a smaller Δt in equation 2.39. When Δt is too small, the required CPU-time will become enormous. To overcome this problem, an implicit formulation is implemented in MT3DMS. See Section 2.6.2.10 for details.

2.6.2.5 MT3DMS/SEAWAT | Species Dependent Diffusion

Select this item to enter diffusion coefficient for individual species. The specified data will be used by MT3DMS or SEAWAT to replace the effective molecular diffusion coefficient in the Dispersion package. The specified data are used only if the Dispersion package is activated.

2.6.2.6 MT3DMS/SEAWAT | Chemical Reaction

The Chemical Reaction package can be used to simulate sorption and chemical reactions. The type of reaction is selected in the Simulation Settings (MT3DMS/SEAWAT) dialog box (Fig. 2.44). The type of sorption and the parameters for sorption and chemical reactions are defined in the the Chemical Reaction (MT3DMS) dialog box (Fig. 2.51) of the Data Editor. The required parameters for the selected sorption and reaction types are summarized below.

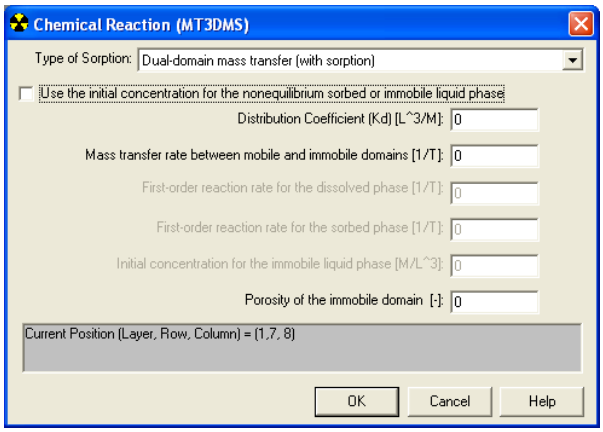

Chemical Reaction (MT3DMS)
Type of Sorption:
Dual-domain mass transfer (with sorption)
Use the initial concentration for the nonequilibrium sorbed or immobile liquid phase
Distribution Coefficient (Kd) [L^3/M]:
0
Mass transfer rate between mobile and immobile domains [1/T]:
0
First-order reaction rate for the dissolved phase [1/T]:
0
First-order reaction rate for the sorbed phase [1/T]:
0
Initial concentration for the immobile liquid phase [M/L^3]:
0
Porosity of the immobile domain [-]:
0
Current Position (Layer, Row, Column) = (1,7, 8)
OK
Cancel
Help

Fig. 2.51. The Chemical Reaction (MT3DMS) dialog box

- *Type of Sorption*: Sorption is implemented in MT3DMS through use of the retardation factor R.

- *No sorption*: Sorption is not simulated.
- *Linear isotherm (equilibrium)* assumes that the sorbed concentration $\overline{C}_{k,i,j}$ is directly proportional to the dissolved concentration $C_{k,i,j}$ (equation 2.42). The retardation factor is therefore independent of the concentration values and is calculated only once for each cell at the beginning of the simulation by equation 2.43.

$$\overline{C}_{k,i,j} = K_d \cdot C_{k,i,j} \tag{2.42}$$

$$R_{k,i,j} = 1 + \frac{\rho_b}{n_{k,i,j}} \cdot K_d \tag{2.43}$$

  where $n_{k,i,j}$ $[-]$ is the porosity of the porous medium in the cell [k, i, j]; K_d $[L^3M^{-1}]$ is the distribution coefficient that depends on the solute species, nature of the porous medium, and other conditions of the system; and ρ_b $[ML^{-3}]$ is the bulk density of the porous medium. The bulk density is the ratio of the mass of dried soil to total volume of the soil.
- *Freundlich isotherm (nonlinear, equilibrium)* is expressed by equation 2.44. The retardation factor at the beginning of each transport step is calculated by equation 2.45.

$$\overline{C}_{k,i,j} = K_f \cdot C^a_{k,i,j} \tag{2.44}$$

$$R_{k,i,j} = 1 + \frac{\rho_b}{n_{k,i,j}} \cdot a \cdot C^{a-1}_{k,i,j} \cdot K_f \tag{2.45}$$

  where $C_{k,i,j}$ is the solute concentration in the cell in the cell [k, i, j] at the beginning of each transport step; a $[-]$ is the Freundlich exponent; and K_f $[L^3M^{-1}]$ is the Freundlich constant.
- *Langmuir isotherm (nonlinear, equilibrium)* is defined by equation 2.46. The retardation factor at the beginning of each transport step is calculated by equation 2.47.

$$\overline{C}_{k,i,j} = \frac{K_L \cdot \overline{S} \cdot C_{k,i,j}}{1 + K_L \cdot C_{k,i,j}} \tag{2.46}$$

$$R_{k,i,j} = 1 + \frac{\rho_b}{n_{k,i,j}} \cdot \frac{K_L \cdot \overline{S}}{\left(1 + K_L \cdot C_{k,i,j}\right)^2} \tag{2.47}$$

  where K_L $[L^3M^{-1}]$ is the Langmuir constant and $\overline{S}$ $[MM^{-1}]$ is the maximum amount of the solute that can be adsorbed by the soil matrix.
- *First-order kinetic sorption (nonequilibrium)*: When the local equilibrium assumption is not valid, MT3DMS assumes that sorption can be represented by a first-order reversible kinetic sorption defined by equation 2.48.

$$\rho_b \cdot \frac{\partial \overline{C}}{\partial t} = \beta \cdot \left(C - \frac{\overline{C}}{K_d} \right) \tag{2.48}$$

  where β $[T^{-1}]$ is the first-order mass transfer rate between the dissolved and sorbed phases; ρ_b $[ML^{-3}]$ is the bulk density of the porous medium; $\overline{C}$ is the sorbed concentration; and K_d $[L^3M^{-1}]$ is the distribution coefficient

that depends on the solute species, nature of the porous medium, and other conditions of the system.
Using the *First-order kinetic sorption* option, the user has the choice of specifying the initial concentration for the sorbed or immobile phase for each species. To do this, simply check "*Use the initial concentration for the nonequibrilium sorbed or immobile liquid phase*" and specify the concentration value to "*Initial concentration for the sorbed phase*" or "*Initial concentration for the immobile liquid phase*" in the Chemical Reaction (MT3DMS) dialog box. If the box "*Use the initial concentration for the nonequibrilium sorbed or immobile liquid phase*" is not checked, it is assumed that the initial concentration of the sorbed or immobile liquid phase is in equilibrium with the initial concentration of the dissolved phase.
Equation 2.48 can be rearranged in

$$C - \frac{\overline{C}}{K_d} = \frac{\rho_b}{\beta} \cdot \frac{\partial \overline{C}}{\partial t} \tag{2.49}$$

If sufficient time is available for the system to reach equilibrium (for example, the flow velocity of groundwater is very slow), then there is no further change in $\overline{C}$ and $\partial \overline{C}/\partial t = 0$, so that equation 2.49 is reduced to linear sorption (equation 2.42). If the first-order mass transfer rate is infinitely large, the right-hand side of equation 2.49 is equal to zero, which also leads to linear sorption. For very small values of β, the left-hand-side of equation 2.48 becomes negligible, i.e., there is no change in the sorbed concentration and sorption is negligible.

– *Dual-domain mass transfer (without sorption)* and *Dual-domain mass transfer (with sorption)*: Dual-domain means that two kinds of continuum, e.g. a fractured medium and the porous medium, exist simultaneously in the same spatial region, i.e., the same model cells. In fractured aquifers, the water moves faster along fractures than it does in a rock formation and the solute transport is often controlled by advection along the fractures and dominated by dispersion in the porous block along the fractures.
MT3DMS uses the dual-domain concept to approach extremely heterogeneous porous media or media composed of fractures and pores. In this approach, the effective porosity specified in *Parameters | Effective Porosity* is used as the primary porosity for the pore spaces filled with mobile water (i.e., fractures) and the secondary porosity for the pore spaces filled with immobile water (i.e., rock formation) is defined in the Chemical Reaction (MT3DMS) dialog box (Fig. 2.51). The sum of the primary and the secondary porosities is the total porosity of the medium. The exchange of solutes between the mobile and immobile domains can be defined through equation 2.50.

$$n_{im} \cdot \frac{\partial C_{im}}{\partial t} = \zeta \cdot (C_m - C_{im}) \tag{2.50}$$

where n_{im} $[-]$ is the secondary porosity (i.e., the portion of total porosity filled with immobile water); C_m $[ML^{-3}]$ is the concentration in the mobile

domain; C_{im} $[ML^{-3}]$ is the concentration in the immobile domain; and ζ $[T^{-1}]$ is the first-order mass transfer rate between the mobile and immobile domains.

As the mass transfer rate ζ increases, the dual-domain model functions more and more like the single-domain model with a porosity approaching the total porosity of the porous medium. For a very small value of ζ, the right-hand-side of equation 2.50 approaches zero, i.e., there is no change of the concentration in the immobile domain and the model functions like a single-porosity model with the primary effective porosity.

One of the advantages of this approach is that the fracture structure does not need to be known. However, a problem may arise when one tries to estimate the mass transfer rate ζ by measuring the concentrations C_m and C_{im}. When the concentration is measured at a certain point, only one value is obtained, which cannot be distinguished between mobile and immobile concentration. It is therefore more likely that ζ must be estimated through a model calibration using C_m values only.

- *Type of Reaction*:
  - *No kinetic reaction is simulated*: reaction is not simulated.
  - *First-order irreversible reaction*: The required parameters are
    * *First-order reaction rate for the dissolved phase* $[1/T]$
    * *First-order reaction rate for the sorbed phase* $[1/T]$

    The concentration change due to the chemical reaction from one transport step to another transport step at cell [k,i,j] can be expressed as

$$\Delta(C_{RCT})_{k,i,j} = -\frac{\Delta t}{R_{k,i,j}} \cdot \left[\lambda_1 \cdot C_{k,i,j} + \lambda_2 \cdot \frac{\rho_b}{n_{k,i,j}} \cdot \overline{C}_{k,i,j}\right] \qquad (2.51)$$

    where λ_1 $[T^{-1}]$ is the first-order rate for the dissolved phase; λ_2 $[T^{-1}]$ is the first-order rate for the sorbed phase; Δt is the transport time-step; and $\overline{C}_{k,i,j}$ is the mass of the solute species adsorbed on the solids per unit bulk dry mass of the porous medium at the beginning of each transport step. $\overline{C}_{k,i,j}$ is in equilibrium with solute concentration $C_{k,i,j}$ in the cell [k,i,j].

    The rate constant λ is usually given in terms of the half-life $t_{1/2}$ (equation 2.55). Generally, if the reaction is radioactive decay, λ_2 should be set equal to λ_1. However, for certain types of biodegradation, λ_2 may be different from λ_1.
  - *Monod kinetics*: MT3D99 implements the Monod kinetics only for the dissolved phase of an organic compound. The required parameters are
    * *Product of total microbial concentration and the maximum specific growth rate of the bacterium* $(M_t \cdot \mu_{max})$ $[ML^{-3}T]$.
    * *Half-Saturation constant* (K_s) $[ML^{-3}]$.

    According to Rifai and others [103] and Zheng [122], the change in the substrate concentration within a transport time-step using the Monod growth function is calculated as follows:

$$\frac{\Delta C}{\Delta t} = M_t \cdot \mu_{max} \cdot \frac{C}{K_s + C} \qquad (2.52)$$

Where C $[ML^{-3}]$ is the substrate concentration; Δt $[T]$ is the length of a transport time-step; M_t $[ML^{-3}]$ is the total microbial concentration; μ_{max} $[T^{-1}]$ is the maximum specific growth rate of the bacterium; and the half-saturation constant K_s $[ML^{-3}]$ represents the substrate concentration at which the rate of growth is half the maximum rate [4].

– *First-order parent-daughter chain reactions*:
The first-order parent-daughter chain reactions is implemented in MT3D99 for both dissolved and sorbed phases. In addition to the yield coefficients between species-pairs (see Section 2.6.2.1), the required parameters for each involved species are
  * *First-order reaction rate coefficient for the dissolved phase* $[T^{-1}]$.
  * *First-order reaction rate coefficient for the sorbed phase* $[T^{-1}]$.

  Considering the dissolved phase, the changes in the concentration values of involved species within a transport time-step are calculated in the following sequential order:

$$\begin{aligned} \frac{\Delta C^1}{\Delta t} &= -\lambda^1 \cdot C^1 \\ \frac{\Delta C^2}{\Delta t} &= -\lambda^2 \cdot C^2 + Y_{1/2}\lambda^1 \cdot C^1 \cdot \\ &\cdots \\ \frac{\Delta C^k}{\Delta t} &= -\lambda^k \cdot C^k + Y_{k-1/k}\lambda^{k-1} \cdot C^{k-1}. \end{aligned} \tag{2.53}$$

  Where C_k $[ML^{-3}]$ is the concentration of species k; Δt $[T]$ is the length of a transport time-step; λ_k $[T^{-1}]$ is the first order reaction rate coefficient for the dissolved phase for species k and $Y_{k-1/k}$ is the yield coefficient between species k-1 and k.

– *Instantaneous reaction among species*: Required stoichiometric ratios between the species are to be specified in the Stoichiometry tab (Fig. 2.45) of the Simulation Settings (MT3DMS/SEAWAT) dialog box in Section 2.6.2.1.

- *Use the initial concentration for nonequilibrium sorbed or immobile liquid phase*: This check box is only used with if the type of sorption is *First-order kinetic sorption (nonequilibrium)*, *Dual-domain mass transfer (without sorption)* or *Dual-domain mass transfer (with sorption)*.
  – For *First-order kinetic sorption (nonequilibrium)*: If this box is checked, the initial concentration of all species for the sorbed phase need to be entered in this dialog box (see below). If this box is cleared, the sorbed phase is assumed to be in equilibrium with the dissolved phase.
  – For *Dual-domain mass transfer*: If this box is checked, the initial concentration of all species for the immobile liquid phase need to be entered in this dialog box (see below). If this box is cleared, the concentration of immobile liquid phase is assumed to be zero.

2.6.2.7 MT3DMS/SEAWAT | Prescribed Fluid Density

The prescribed fluid density is used by SEAWAT if the simulation mode is set as *Variable Density Flow and Transport with SEAWAT* and the density-effect of all the simulated species is turned off. Refer to the Species tab of Section 2.6.2.1 for details.

2.6.2.8 MT3DMS/SEAWAT | Sink/Source Concentration

This menu is used for specifying the concentration associated with the fluid of point or spatially distributed sources or sinks. The concentration value of a particular source or sink is specified in the Data Editor. Point sources include wells, general head boundary cells, fixed-head cells, rivers and streams. Recharge is the only spatially distributed source whereas evapotranspiration is the only sink whose concentration can be specified. The concentration of a sink cannot be greater than that of the groundwater at the sink cell. If the sink concentration is specified greater than that of the groundwater, it is automatically set equal to the concentration of the groundwater. Therefore, setting a big sink concentration value (e.g. 1×10^{30}) to evapotranspiration ensures that the groundwater concentration is used for the computation.

Note that MT3DMS does not allow the concurrent use of the rivers and the streams. This does not cause problems in any case, because the Streamflow Routing package has all functions of the River package.

Menu items of this menu are dimmed if the corresponding hydraulic features given in the *Models* | *MODFLOW* menu are not used (checked). The user may or may not specify the concentration for the sources or sinks when they are used in the flow simulation. The specified concentration will be used in the transport simulation if a corresponding menu item is checked. If a checked item is no longer necessary for a transport simulation, simply select the item again and deactivate it. If the concentration of a source or sink is not specified, the default value for the concentration is zero.

Using the menu item Time Variant Specified Concentration, the user may define constant concentration cells anywhere in the model grid and different concentration values may be specified for different stress periods. A time varying specified concentration cell is defined by setting the following data in the Data Editor.

- *Flag* $[-]$. A non zero value indicates that a cell is specified as a constant concentration cell. In a multiple stress period simulation, a constant-concentration cell, once defined, remains a constant-concentration cell during the simulation, but its concentration value can be specified to vary in different stress period. To change the concentration value in a particular stress period, simply set a non-zero value to Flag and assign the desired concentration value to Specified Concentration. **In a multispecies simulation, the Flag is applied to all species.**
- *Specified Concentration* $[ML^{-3}]$. This value is the concentration in the cell from the beginning of a stress period. If the constant-concentration condition does not apply to a particular species, assign a negative concentration value for that species. The negative value is used by MT3DMS to skip assigning the constant-concentration for the designated species.

2.6.2.9 MT3DMS/SEAWAT | Mass-Loading Rate

Instead of specifying a source concentration associated with a fluid source, the mass-loading rate $[MT^{-1}]$ into the groundwater system can directly be specified by using this menu item. This is of interest for example for the case where dissolution of an oil spill occurs and the groundwater flowing through the residually saturated oil body picks up hydrocarbons.

2.6.2.10 MT3DMS/SEAWAT | Solver | GCG

MT3DMS includes a general-purpose iterative solver based on the generalized conjugate gradient method for solving the system of the transport equations. The solver is implemented in the Generalized Conjugate Gradient package. A detailed description of the method can be found in Zheng and Wang [121].

This solver must always be activated. Using this solver, dispersion, sink/source, and reaction terms are solved implicitly without any stability constraints on the transport step size. The required settings and parameters for this package are specified in the Generalized Conjugate Gradient (GCG) dialog box (Fig. 2.52).

- *Preconditioning Method*: The GCG package has three preconditioning options, Jacobi, Symmetric Successive Overrelaxation (SSOR), and the Modified Incomplete Cholesky (MIC). The MIC preconditioner usually takes less iterations than the other methods, but it requires significantly more memory.
- *Max. Number of Outer Iterations (MXITER)*and *Max. Number of Inner Iterations (ITER1)*: The GCG solver has two iteration loops, an inner loop and an outer loop. Like the PCG2 solver of MODFLOW (see page 65), within the inner loop all coefficients in the (transport-) matrix $\underline{A}$ and the right-hand-side vector ($\underline{b}$) remain unchanged during inner iterations. The inner loop continues until ITER1 - iterations are executed or the convergence criterion is met. If some of the coefficients in $\underline{A}$ are dependent on the concentration being solved, as in the case of nonlinear sorption, they must be updated in outer iterations. So, MXITER should be set to an integer greater than one only when a nonlinear sorption isotherm is included in the simulation. For ITER1, a value between 30 and 50 should be adequate for most problems.

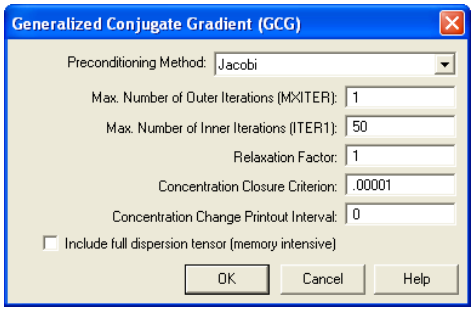


Fig. 2.52. The Generalized Conjugate Gradient (GCG) dialog box

- *Relaxation Factor* is only used for the SSOR option; a value of 1.0 is generally adequate.
- *Concentration Closure Criterion is the convergence criterion*; a value between 10^{-6} and 10^{-4} is generally adequate. Before solving the system of transport equations, it is normalized by dividing the concentration terms by the maximum concentration of all cells. When the change of the normalized concentration at all cells during a inner iteration is less than or equal to this value, iteration stops. When it takes only one inner iteration to converge, the solution is considered to have converged and the simulation proceeds to the next transport step.
- *Concentration Change Printout Interval*: The maximum concentration changes are printed out whenever the iteration number is an even multiple of this printout interval. Set it to zero for printing only at the end of each stress period.
- *Include full dispersion tensor (memory intensive)*: This is a flag for treatment of dispersion tensor cross terms. If this option is not used, all dispersion cross terms will be lumped to the right-hand-side of the system of transport equations. Omitting the cross terms represents a method of approximation, which is highly efficient. It must be noted, however, that for critical applications the full dispersion tensor should be included.

2.6.2.11 MT3DMS/SEAWAT | Concentration Observations

Select this menu item from the MT3DMS menu (or from MOC3D, MT3D, or RT3D) to specify the locations of the concentration observation boreholes and their associated observed (measurement) data in a Concentration Observations dialog box. Its use is identical to the Head Observation dialog box (see Section 2.6.1.14). The only difference is that the head observations are replaced by concentration observations.

2.6.2.12 MT3DMS/SEAWAT | Output Control

Use the Output Control (MT3D/MT3DMS) dialog box (Fig. 2.53) to set the output options of MT3D. The options in this dialog box are grouped under three tabs described below.

- *Output Terms*: The MT3DMS transport model always generates a listing file OUTPUT.MTM, which documents the details of each simulation step. Optionally, you can save other output terms by checking the corresponding output terms in this tab. All output terms denoted by (ASCII) are also saved in the listing file. The calculated dissolved-phase concentration values are saved in the unformatted binary files MT3D*nnn*.UCN, where *nnn* is the species number. The calculated sorbed-phase or immobile-liquid phase concentration values are saved in the unformatted binary files MT3D*nnn*S.UCN All output files are located in the same folder as your model. You can use the Result Extractor to read the unformatted binary files.
- *Output Times*: The value of the output frequency, NPRS, indicates whether the output is produced in terms of total elapsed simulation time or the transport step

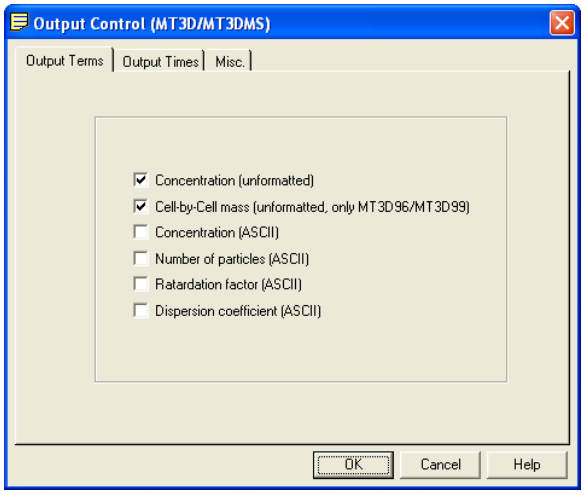


Fig. 2.53. The Output Control (MT3D/MT3DMS) dialog box

number. If NPRS=0, simulation results will only be saved at the end of simulation. If NPRS < 0, simulation results will be saved whenever the number of transport steps is an even multiple of NPRS. If NPRS > 0, simulation results will be saved at times as specified in the table shown in Fig. 2.54. There are two ways for specifying the output times. The user may click the table header Output Time and then enter a minimum time, a maximum time and a time interval between each output into an Output Time dialog box. **PM** will use these entries to calculate NPRS and the output times. The other way is to specify a positive NPRS and press the Tab key, then enter the output times into the table. Note that the output times are measured from the beginning of the simulation.

- *Misc.*:
  - *CINACT* is the predefined concentration value for an inactive concentration cell (ICBUND = 0). This value is a marker for these cells only and has no physical meaning.
  - *THKMIN* is the minimum saturated thickness in a cell, expressed as the decimal fraction of the model layer thickness, below which the cell is considered inactive.
  - *NPRMAS* indicates how frequently the mass budget information should be saved in the mass balance summary file MT3D*nnn*.MAS, where *nnn* is the species number.

2.6.2.13 MT3DMS/SEAWAT | Run

If the *Simulation Mode* is set as *Constant Density Transport with MT3DMS*, the Run MT3DMS dialog box (Fig. 2.55) will be displayed. If the *Simulation Mode* is set as *Variable Density and Transport with SEAWAT*, the Run SEAWAT dialog box (Fig. 2.56) will be displayed in place of the Run MT3DMS dialog box.

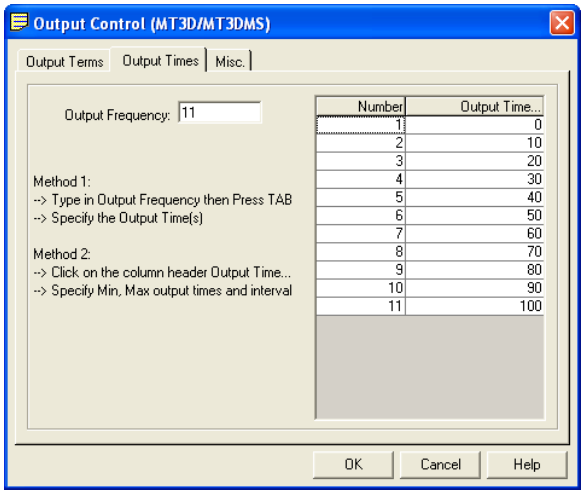


Fig. 2.54. The Output Times tab of the Output Control (MT3D/MT3DMS) dialog box

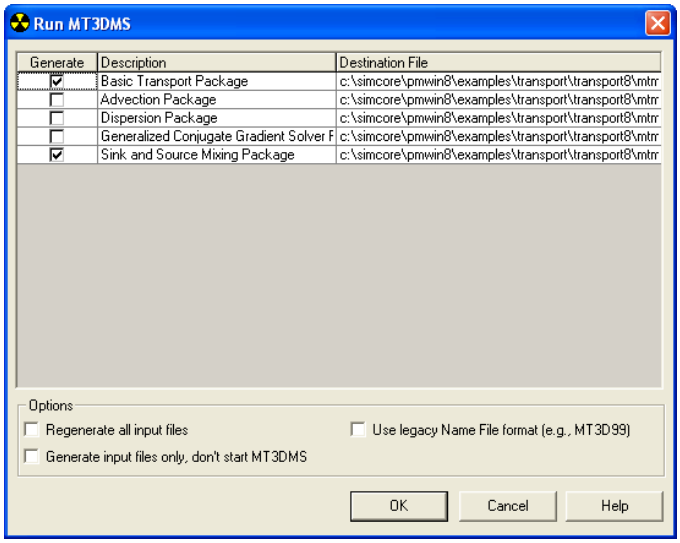


Fig. 2.55. The Run MT3DMS dialog box

Run MT3DMS dialog box: The available settings of the Run MT3DMS dialog box are described below.

- The File Table has three columns:
  - *Generate*: Prior to running a transport simulation, **PM** uses the user-specified data to generate input files for MT3DMS. An input file will be generated if it does not exist or if the corresponding *Generate* box is checked. Normally,

we do not need to worry about these boxes since **PM** will take care of the settings.
  - *Description* gives the names of the packages used in the model.
  - *Destination File* shows the paths and names of the input files of the model.
- Options:
  - *Regenerate all input files*: Check this option to force **PM** to generate all input files regardless the setting of the Generate boxes. This is useful if the input files have been deleted or overwritten by other programs.
  - *Generate input files only, don't start MT3DMS*: Check this option, if the user does not want to run MT3DMS. The simulation can be started at a later time or can be started at the Command Prompt (DOS box) by executing the batch file MT3DMS.BAT.
  - *Use Legacy Name File Format, e.g., MT3D99*: The Name File of later versions of MT3DMS uses the same format as MODFLOW-2000. However, old versions of MT3D, MT3DMS and its variants such as MT3D99 use an older format. Check this box, if you are running MT3D99 or older versions of MT3DMS.
- *OK*: Click *OK* to generate MT3DMS input files. In addition to the input files, **PM** creates a batch file MT3DMS.BAT in the model folder. When all input files are generated, **PM** automatically runs MT3DMS.BAT in a Command Prompt-window (DOS box). During a simulation, MT3DMS writes a detailed run record to the file OUTPUT.MTM saved in the model folder. See Section 2.6.2.12 on page 104 for details about the output terms.

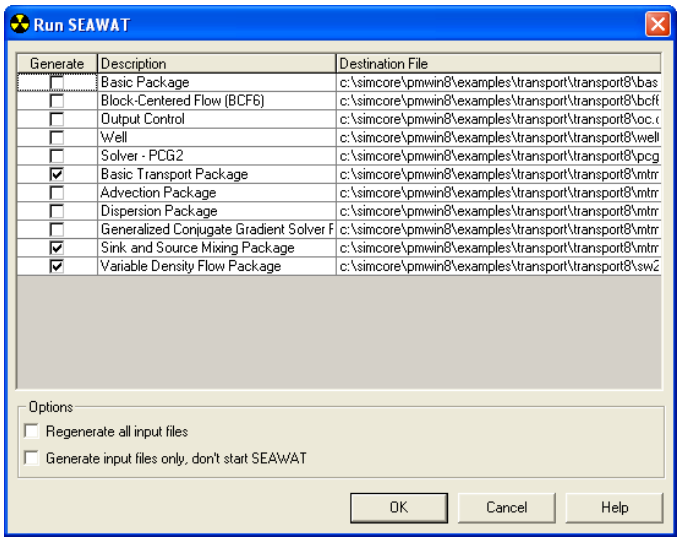


Fig. 2.56. The Run SEAWAT dialog box

Run SEAWAT dialog box: The available settings of the Run SEAWAT dialog box are described below.

- The File Table has three columns:
  - *Generate*: Prior to running a transport simulation, **PM** uses the user-specified data to generate input files for SEAWAT. An input file will be generated if it does not exist or if the corresponding *Generate* box is checked. Normally, we do not need to worry about these boxes since **PM** will take care of the settings.
  - *Description* gives the names of the packages used in the model.
  - *Destination File* shows the paths and names of the input files of the model.
- Options:
  - *Regenerate all input files*: Check this option to force **PM** to generate all input files regardless the setting of the Generate boxes. This is useful if the input files have been deleted or overwritten by other programs.
  - *Generate input files only, don't start SEAWAT*: Check this option, if the user does not want to run SEAWAT. The simulation can be started at a later time or can be started at the Command Prompt (DOS box) by executing the batch file SEAWAT.BAT.
- *OK*: Click *OK* to generate SEAWAT input files. In addition to the input files, **PM** creates a batch file SEAWAT.BAT in the model folder. When all input files are generated, **PM** automatically runs SEAWAT.BAT in a Command Prompt-window (DOS box). During a simulation, SEAWAT writes a detailed run record to the file OUTPUT.SWT saved in the model folder. See Section 2.6.2.12 on page 104 for details about the output terms.

2.6.2.14 MT3DMS/SEAWAT | View

MT3DMS/SEAWAT | View | Run Listing File

Select this menu item to use the Text Viewer (see Section 2.3.4) to display the run list file OUTPUT.MTM of MT3DMS or OUTPUT.SWT of SEAWAT, which contains a detailed run record saved by MT3DMS or SEAWAT, respectively.

MT3DMS/SEAWAT | View | Concentration Scatter Diagram

This menu item is available only if Concentration Observations have been defined (see Section 2.6.2.11 on page 104). Select this menu item to open a Scatter Diagram (Concentration) dialog box, which is identical to the Scatter Diagram (Hydraulic Head) dialog box (Fig. 2.38 on page 78), except the concentration values replace the head values.

MT3DMS/SEAWAT | View | Concentration-Time Curves

This menu item is available only if Concentration Observations have been defined (see Section 2.6.2.11 on page 104). Select this menu item to open a Time Series Curves (Concentration) dialog box, which is identical to the Time Series Curves (Hydraulic Head) dialog box (Fig. 2.41 on page 82), except the concentration values replace the head values.

2.6.3 PHT3D

With the exception of user-definable reaction modules that use PHREEQC-2 as the reaction simulator, the PHT3D interface of **PM** is identical to the MT3DMS/SEAWAT interface with the *Simulation Mode* setting to *Constant Density Transport with MT3DMS* (see Section 2.6.2.1).

As is the case with MT3DMS, the composition of a PHT3D model starts with *Simulation Settings* and PHT3D simulations are carried out on the basis of flow-fields computed beforehand by MODFLOW. Thus, as given by Prommer and others [97], PHT3D cannot reproduce the potential impact of reactive processes on the groundwater flow field and the model is not suitable to predict, for example, the impact of bioclogging or mineral precipitation on the hydraulic properties of an aquifer. The simultaneous use of the MT3DMS chemical reaction package (RCT) and PHREEQC-2 as reaction simulator(s) is possible. However, this should be done with appropriate care, i.e., control of potential operator-splitting errors.

2.6.3.1 PHT3D | Simulation Settings

The simulation settings of PHT3D are completed in two dialog boxes. The Chemical Reaction Module (PHT3D) dialog box (Fig. 2.57) will appear first allowing the user to select a pre-defined chemical reaction module. For simpler problems, such as those that only include equilibrium reactions, all of the aqueous species, components and minerals are already included in the original *PHREEQC-2 Standard database*. In addition, **PM** includes more than 10 reaction modules from PHT3D examples. See Section 5.6 for a complete list of PHT3D examples. In some cases a problem-specific reaction module needs to be prepared and added to **PM** before using PHT3D. See Section 6.5 for the steps of defining a customized reaction module.
Once a reaction module is selected and the Chemical Reaction Module (PHT3D) dialog box is closed, the Simulation Settings (PHT3D) dialog box (Fig. 2.58) appears. The tabs of the dialog box are described below.

- *Component (equilibrium)*: This tab contains a table and each row of the table defines an aqueous component that are assumed to be in chemical equilibrium. The columns of the table are defined as follows.
  - *Active*: Check the box to include the respective component in the simulation. A transport simulation will be carried out for each of the included aqueous components, except for pH and pe. As pH and pe are included in all simulation, they cannot be deactivated.
  - *Component*: Name of the component.

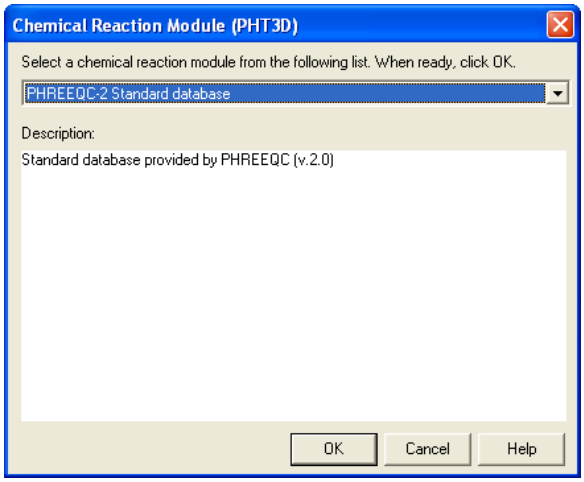


Fig. 2.57. The Chemical Reaction Module (PHT3D) dialog box

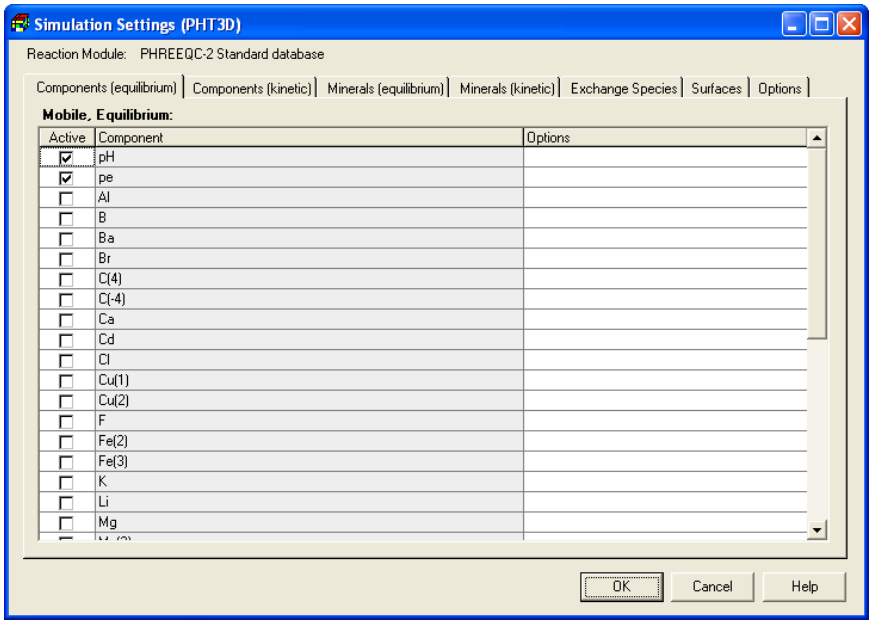


Fig. 2.58. The Simulation Settings (PHT3D) dialog box

  - *Options*: This is an optional argument that is passed to the PHREEQC-2 input file to take advantage of the numerous options in PHREEQC to define concentration values. For example, the charge option can be invoked, or the option to calculate the input concentration of an element from equilibrium with a pure phase. See the PHREEQC-2 manual [91] for more details.
- *Component (kinetic)*: This tab contains two tables that define mobile kinetic reactants and immobile kinetic reactants, respectively. For each reactant, a rate expression is defined in the database-file of the selected reaction module and the local equilibrium assumption is assumed to be invalid. The columns of the tables are defined as follows.
  - *Active*: Check the box to include the respective reactant in the simulation.
  - *Component*: Name of the reactant.
  - *Stoichiometry*: Stoichiometry is expressed in the form of "*reactant1 -mole_r1 reactant2 -mole_r2... product1 mole_p1 product2 mole_p2*", and is pre-defined in the database-file of the selected reaction module.
  - *Parm 1 to 8*: Parameters used to define the reaction rate. The parameters are pre-defined in the database-file of the selected reaction module.
- *Minerals (equilibrium)*: Each row of the table contains a mineral for which the local equilibrium assumption (LEA) is assumed to be valid. Check the *Active* of a row to include the respective mineral in the simulation. No transport step is carried out for minerals. The columns of the table are defined as follows.
  - *Active*: Check the box to include the respective mineral in the simulation.
  - *Mineral*: Name of the mineral.
  - *Options*: This is an optional argument that can be entered for each of the minerals that are included in a simulation. This value represents the target Saturation Index (SI) for a pure phase in the aqueous phase.
  - *Equation*: This column contains the exact definitions of the minerals.
- *Minerals (kinetic)*: Each row of the table contains a mineral for which a rate expression is defined in the database-file of the selected reaction module and the local equilibrium assumption is assumed to be invalid. The columns of the table are defined as follows.
  - *Active*: Check the box to include the respective mineral in the simulation.
  - *Mineral*: Name of the mineral.
  - *Stoichiometry*: Stoichiometry is expressed in the form of "*reactant1 -mole_r1 reactant2 -mole_r2... product1 mole_p1 product2 mole_p2*", and is pre-defined in the database-file of the selected reaction module.
  - *Parm 1 to 8*: Parameters used to define the reaction rate. The parameters are pre-defined in the database-file of the selected reaction module.
- *Exchange Species*: Each row of the table contains an exchange species involved in cation-exchanging reactions with an exchanger.
  The columns of the table are defined as follows.
  - *Active*: Check the box to include the respective species in the simulation.
  - *Exchange Species*: Name of the exchange species.

- *Surfaces*:
  The dropdown box *Surface Complexation Model* contains the information on which type of SCM calculation will be executed by PHREEQC. Each row of the table contains a *Surface Master Species* defined in the database-file of the selected reaction module.
  - *Active*: Check the box to include the respective surface master species in the simulation.
  - *Surface Master Species*: The name of surface master species.
  - *Surface Area* defines the specific surface area of a surface, either in m^2/g (when the number of sites and mass of a surface are entered explicitly) or in m^2/mol (when the amount of surface sites is coupled to a pure phase or a kinetic reactant).
  - *Mass* defines the mass of solid and is used to calculate the surface area. Although a value must always be specified here, it is only used when the number of sites and mass are defined explicitly, i.e., when not coupled to a pure phase or kinetic reactant.
  - *Phase/Reactant* + *Switch*: *Phase/Reactant* is an optional argument to define a pure phase or kinetic reactant to which the surface binding site must be coupled. The number of moles of surface sites will be calculated from the number of moles of the phase/reactant. *SWITCH* is an optional argument to define whether a pure phase is used (Phase/Reactant = equilibrium phase) or a kinetic reactant (Phase/Reactant = kinetic reactant). Phase/Reactant only works in conjunction with *Phase/Reactant*, that is, there is no need to specify it unless *Phase/Reactant* is defined. If no value is specified the default is equilibrium phase.
- *Options*:
  - *Simulation Options*
    * *Temperature of the aqueous solution* is is the temperature in Celsius used in chemical reactions for which a temperature dependence is defined in the database file. The default value is 25C.
    * *Output File Format* determines ASCII files (extension .ACN) and/or Binary files (.UCN) that contain the computed concentrations for all grid-cells and for all output times that are defined in the *PHT3D | Output Control*.
    * *CB_OFFSET* is a number that acts as a flag to indicate if the charge imbalance carried by a solution is to be transported. If CB_OFFSET ¿ 0, the charge imbalance of solutions is transported. This is achieved by adding CB_OFFSET to the charge imbalance of all solution. The resulting values are used as the "concentrations" in the transport equations to calculate the redistribution of the charge imbalance.If CB_OFFSET = 0, the charge imbalance is not transported. Default value for CB_OFFSET is 0.05.
  - *Threshold values for executing PHREEQC*
    * *Changes in aqueous concentration values* is the PHREEQC-2 activation/deactivation criteria as described in the PHT3D manual. At the be-

ginning of each reaction step, PHT3D checks for each cell by which amount the concentration of the mobile species have changed during the previous reaction step. If the change in a cell is smaller than *Changes in aqueous concentration values*, no reactions are calculated for that cell. The user should always verify that the selected value has negligible effect on the simulation outcome. If the value is set to 0, PHREEQC-2 will be executed for all grid-cells (except fixed concentration boundaries) in all reaction steps.

* *Changes in pH* is the PHREEQC-2 activation/deacvtivation as described in the PHT3D manual. This value is only used when greater than zero and when *Changes in aqueous concentration values* is greater than zero.

2.6.4 RT3D

2.6.4.1 RT3D | Simulation Settings

The available settings of the Reaction Definition (RT3D) dialog box (Fig. 2.59) are described below.

- *Reaction Module*: Currently seven pre-programmed reaction modules are available. Their purposes, taken from the RT3D manual, are described briefly below. Refer to Clement [25] for their reaction algorithms.
  - *No Reaction (tracer transport)*: chemical reaction is not simulated.
  - *Instantaneous aerobic decay of BTEX*: Simulates aerobic degradation of BTEX using an instantaneous reaction model. The reaction simulated are similar to those simulated by BIOPLUME-II [102].
  - *Instantaneous degradation of BTEX using multiple electron acceptors*: Simulates instantaneous biodegradation of BTEX via five different degradation

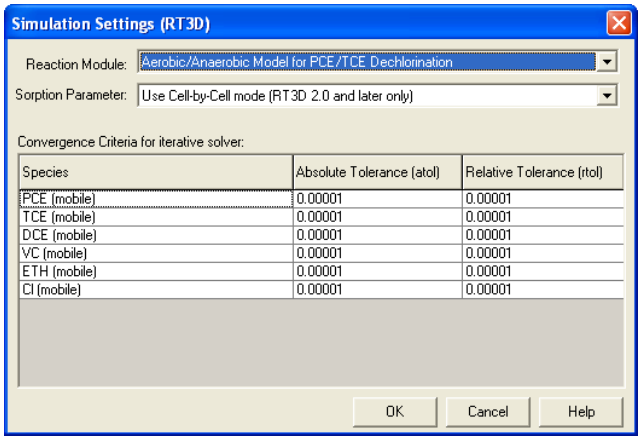


Fig. 2.59. The Reaction Definition (RT3D) dialog box

pathways: aerobic respiration (O_2), denitrification (NO_3^-), iron reduction (Fe^{2+}), sulfate reduction (SO_4^{2-}), and methanogenesis (CH_4).
  - *Kinetic-limited degradation of BTEX using multiple electron acceptors*: Simulates kinetic-limited biodegradation of BTEX via five different degradation pathways: aerobic respiration (O_2), denitrification (NO_3^-), iron reduction (Fe^{2+}), sulfate reduction (SO_4^{2-}), and methanogenesis (CH_4).
  - *Rate-limited sorption reactions*: Simulates first-order reversible kinetic sorption. This option is equivalent to "First-order kinetic sorption" in the chemical reaction package of the MT3DMS (*Models* | *MT3DMS/SEAWAT* | *Chemical Reaction*).
  - *Double Monod model*: Simulates the reaction between an electron donor and an electron acceptor mediated by actively growing bacteria cells living in both aqueous and soil phases.
  - *Sequential decay reactions*: Simulates reactive transport coupled by a series of sequential degradation reactions (up to four components) under anaerobic conditions.
  - *Anaerobic and aerobic biodegradation of PCE/TCE/DCE/VC*: Simulates sequential degradation of perchloroethene (PCE) → trichloroethene (TCE) → dichloroethene (DCE) → vinyl chloride (VC) via both aerobic and anaerobic paths.
- *Sorption Parameter*: Defines whether the sorption parameters are going to be specified layer-by-layer (Use Layer-by-Layer mode) or cell-by-cell (Use Cell-by-Cell mode). The latter can only be used by RT3D version 2.0 or later. The sorption parameters are specified using *Models* | *RT3D* | *Sorption Parameters*.
- *Convergence Criteria for iterative solver*: The table contains a list of species for the selected reaction module. Reaction solvers of RT3D use absolute tolerance (atol) and relative tolerance (rtol) values to control convergence errors. The following rule of thumb may be used to set the atol and rtol values. If m is the number of significant digits required in a solution component, set rtol = $10^{-(m+1)}$ and set atol to a small value at which the absolute value of the component is essentially insignificant. Note that the values of atol and rtol should always be positive.

2.6.4.2 RT3D | Initial Concentration

At the beginning of a transport simulation, RT3D requires the initial concentration of each active species at each active concentration cell, i.e. ICBUND > 0.

2.6.4.3 RT3D | Advection

Select this menu item to open an Advection Package (RT3D) dialog box. The use of this dialog box is identical to the Advection Package (MT3DMS) dialog box (Fig. 2.47 on page 90).

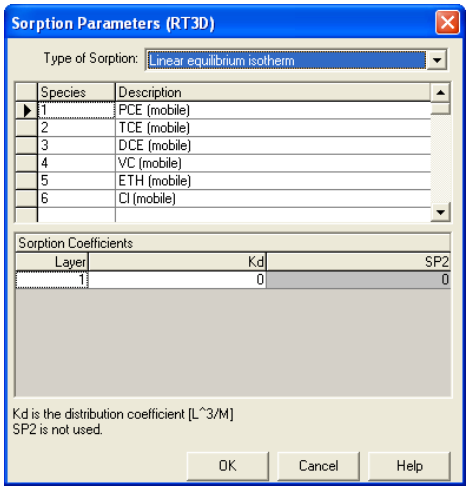


Fig. 2.60. The Sorption Parameters (RT3D) dialog box

2.6.4.4 RT3D | Dispersion

Select this menu item to open a Dispersion Package dialog box. Its use is identical to the Dispersion Package of MT3DMS, see Section 2.6.2.4 for details.

2.6.4.5 RT3D | Sorption | Layer by Layer

This menu item is available only if *Sorption Parameter* of the Simulation Settings (RT3D) dialog box (see Section 2.6.4.1) is set to *Use Layer-by-Layer mode*. The available settings of the Sorption Parameters (RT3D) dialog box (Fig. 2.60) are given below.

- *Type of Sorption*: RT3D supports three sorption types, i.e., linear equilibrium isotherm, Freundlich nonlinear equilibrium isotherm, and Langmuir nonlinear equilibrium isotherm. See Section 2.6.2.6 for details.
- *Species*: Select a species, for which the sorption coefficients are to be specified.
- *Sorption Coefficients*: Use this table to specify the required parameters on a layer-by-layer basis. Refer to Section 2.6.6.4 for details about the sorption coefficients.

2.6.4.6 RT3D | Sorption | Cell by Cell

This menu item is available only if Sorption Parameter of the Simulation Settings (RT3D) dialog box (see Section 2.6.4.1) is set to *Use Cell-by-Cell mode (RT3D 2.0 and later only)*. Using the Data Editor, sorption coefficients may be entered on a three dimensional cell by cell basis. This option provides the ability to have different coefficients for different areas.

2.6.4.7 RT3D | Reaction Parameters | Spatially Constant

In RT3D, reaction parameter values of each species can be spatially constant for the entire model or can be variable from cell to cell. Select this menu item to assign spatially constant parameter values to the Reaction Parameters for RT3D (Spatially Constant) dialog box (Fig. 2.61).

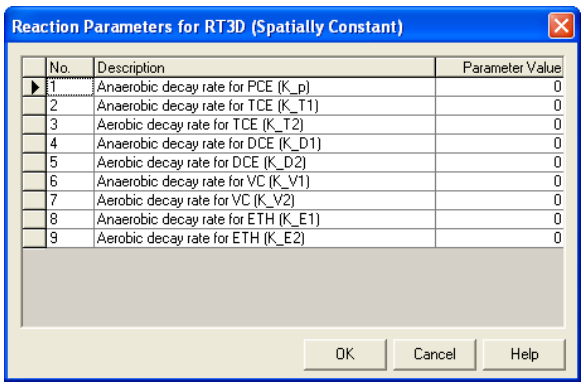

Reaction Parameters for RT3D (Spatially Constant)
No.
Description
Parameter Value
1 Anaerobic decay rate for PCE (K_p) 0
2 Anaerobic decay rate for TCE (K_T1) 0
3 Aerobic decay rate for TCE (K_T2) 0
4 Anaerobic decay rate for DCE (K_D1) 0
5 Aerobic decay rate for DCE (K_D2) 0
6 Anaerobic decay rate for VC (K_V1) 0
7 Aerobic decay rate for VC (K_V2) 0
8 Anaerobic decay rate for ETH (K_E1) 0
9 Aerobic decay rate for ETH (K_E2) 0
OK
Cancel
Help

Fig. 2.61. The Reaction Parameters for RT3D (Spatially Constant) dialog box

2.6.4.8 RT3D | Reaction Parameters | Spatially Variable

Select this menu item to specify spatially variable (cell-by-cell) reaction parameters. Note that this menu item cannot be used if the Reaction Module in the Simulation Settings (RT3D) dialog box (Fig. 2.59) is one of the following: *No Reaction (tracer transport)*, *Instantaneous aerobic decay of BTEX*, or *Instantaneous degradation of BTEX using multiple electron acceptors*.

2.6.4.9 RT3D | Sink/Source Concentration

The use of this menu is the same as *MT3D | Sink/Source Concentration*, except the use of the menu item *Time-Variant Specified Concentration*. A time varying specified concentration cell is defined by setting the following data in the Data Editor.

- *Flag* [−]. A non zero value indicates that a cell is specified as a constant concentration cell. In a multiple stress period simulation, a constant-concentration cell, once defined, remains a constant-concentration cell during the simulation, but its concentration value can be specified to vary in different stress period. To change the concentration value in a particular stress period, simply set a non-zero value to Flag and assign the desired concentration value to Specified Concentration. **In a multispecies simulation, the Flag is applied to all species.**

- *Specified Concentration* $[ML^{-3}]$. This value is the concentration in the cell from the beginning of a stress period. If the constant-concentration condition does not apply to a particular species, assign a negative concentration value for that species. The negative value is used by RT3D to skip assigning the constant-concentration for the designated species.

2.6.4.10 RT3D | Concentration Observations

Select this menu item from the RT3D menu (or from MOC3D, MT3DMS, or MT3D) to specify the locations of the concentration observation boreholes and their associated observed (measurement) data in a Concentration Observations dialog box. Its use is identical to the Head Observation dialog box (see Section 2.6.1.14). The only difference is that the head observations are replaced by concentration observations.

2.6.4.11 RT3D | Output Control

The output control of RT3D is the same as that of MT3DMS/SEAWAT. See Section 2.6.2.12 on page 104 for details.

2.6.4.12 RT3D | Run

The available settings of the Run RT3D dialog box (Fig. 2.62) are described below.

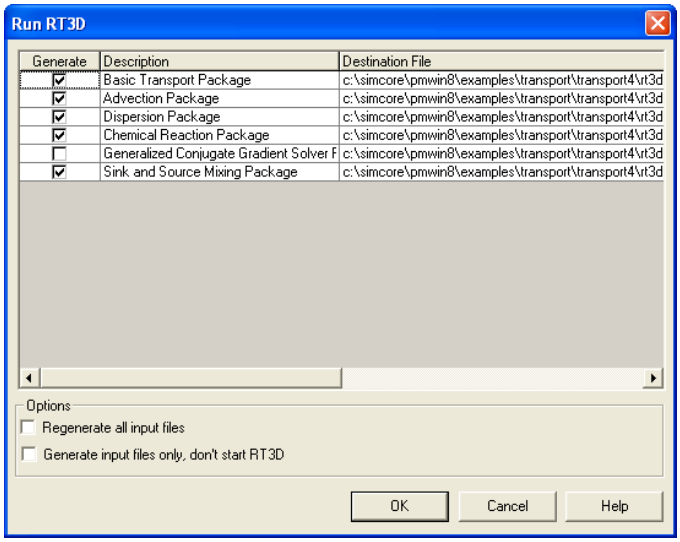


Fig. 2.62. The Run RT3D dialog box

- The File Table has three columns:

  - *Generate*: Prior to running a transport simulation, **PM** uses the user-specified data to generate input files for RT3D. An input file will be generated if it does not exist or if the corresponding *Generate* box is checked. The user may click on a box to check or clear it. Normally, we do not need to worry about these boxes since **PM** will take care of the settings.
  - *Description* gives the names of the packages used in the model.
  - *Destination File* shows the paths and names of the input files of the model.
- Options:
  - *Regenerate all input files*: Check this option to force **PM** to generate all input files regardless the setting of the Generate boxes. This is useful if the input files have been deleted or overwritten by other programs.
  - *Generate input files only, don't start RT3D*: Check this option, if the user does not want to run RT3D. The simulation can be started at a later time or can be started at the Command Prompt (DOS box) by executing the batch file RT3D.BAT.
- *OK*: Click *OK* to start generating RT3D input files. In addition to the input files, **PM** generates a batch file MT3DMS.BAT saved in the model folder. When all necessary files are generated, **PM** automatically runs RT3D.BAT in a Command Prompt-window (DOS box). During a simulation, RT3D writes a detailed run record to the file OUTPUT.RT3 saved in the model folder. See Section 2.6.2.12 on page 104 for details about the output terms.

2.6.4.13 RT3D | View

RT3D | View | Run Listing File

Select this menu item to use the Text Viewer (see Section 2.3.4) to display the run list file OUTPUT.MTM, which contains a detailed run record saved by MT3DMS.

RT3D | View | Concentration Scatter Diagram

This menu item is available only if Concentration Observations have been defined (see Section 2.6.4.10 on page 117). Select this menu item to open a Scatter Diagram (Concentration) dialog box, which is identical to the Scatter Diagram (Hydraulic Head) dialog box (Fig. 2.38 on page 78), except the concentration values replace the head values.

RT3D | View | Concentration-Time Curves

This menu item is available only if Concentration Observations have been defined (see Section 2.6.4.10 on page 117). Select this menu item to open a Time Series Curves (Concentration) dialog box, which is identical to the Time Series Curves (Hydraulic Head) dialog box (Fig. 2.41 on page 82), except the concentration values replace the head values.

2.6.5 MOC3D

2.6.5.1 MOC3D | Subgrid

Within the finite-difference grid used to solve the flow equation in MODFLOW, the user may specify a window or subgrid over which MOC3D will solve the solute-transport equation. This feature can significantly enhance the overall efficiency of the model by avoiding calculation effort where it is not needed. However, MOC3D requires that within the area of the transport subgrid, row and column discretization must be uniformly spaced (that is, x and y must be constant, although they need not be equal to each other). The spatial discretization or rows and columns beyond the boundaries of the subgrid can be nonuniform, as allowed by MODFLOW, to permit calculations of head over a much larger area than the area of interest for transport simulation. Vertical discretization, defined by the cell thickness, can be variable in all three dimensions. However, large variability may adversely affect numerical accuracy. For details, refer to Konikow et al. [74] for the model assumptions that have been incorporated into the MOC3D model.

The subgrid is defined in the Subgrid for Transport (MOC3D) dialog box (Fig. 2.63). MOC3D assumes that the concentration outside of the subgrid is the same within each layer, so only one concentration value is specified for each layer within or adjacent to the subgrid by using the *C' Outside of Subgrid* table of this dialog box. The values of other layers, which are not within or adjacent to the subgrid, are ignored.

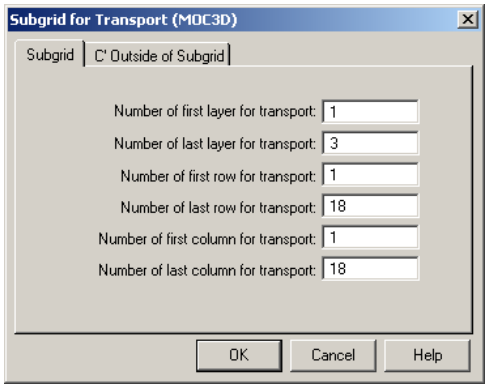

Subgrid for Transport (MOC3D)
Subgrid
C' Outside of Subgrid
Number of first layer for transport: 1
Number of last layer for transport: 3
Number of first row for transport: 1
Number of last row for transport: 18
Number of first column for transport: 1
Number of last column for transport: 18
OK
Cancel
Help

Fig. 2.63. The Subgrid for Transport (MOC3D) dialog box

2.6.5.2 MOC3D | Initial Concentration

MOC3D requires initial concentration of each cell within the transport subgrid at the beginning of a transport simulation. The values specified here are shared with MT3D.

2.6.5.3 MOC3D | Advection

Use the Parameter for Advective Transport (MOC3D) dialog box (Fig. 2.64) to specify the required data as described below.

- *Interpolation scheme for particle velocity*: In MOC3D, the advection term of a solute transport process is simulated by the Method of Characteristics (MOC). Using the MOC scheme, a set of moving particles is distributed in the flow field at the beginning of the simulation. A concentration and a position in the Cartesian coordinate system are associated with each of these particles. Particles are tracked forward through the flow field using a small time increment. At the end of each time increment, the average concentration at a cell due to advection alone, is evaluated from the concentrations of particles, which happen to be located within the cell. The other terms in the governing equation, i.e. dispersion, chemical reaction and decay, are accounted for by adjusting the concentrations associated with each particle after the redistribution of mass due to those processes on the grid.
  A moving particle in a ground-water flow system will change velocity as it moves due to both spatial variation in velocity and temporal variations during transient flow. During a flow time step, advection is determined from velocities computed at the end of the flow time step. Temporal changes in velocity are accounted for by a step change in velocity at the start of each new flow time step. After the flow equation is solved for a new time step, the specific discharge across every face of each finite-difference cell is recomputed on the basis of the new head distribution, and the movement of particles during this flow time step is based only on these specific discharges.
  MOC3D provides two interpolation options - linear and bilinear interpolation, for calculating the spatial variation of the particle velocity from the specific discharges. Konikow and others [74] indicate that if transmissivity within a layer is homogeneous or smoothly varying, bilinear interpolation of velocity yields more

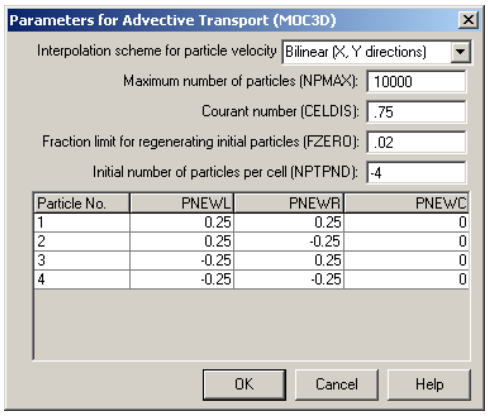


Fig. 2.64. The Parameter for Advective Transport (MOC3D) dialog box

realistic pathlines for a given discretization than linear interpolation. And, in the presence of strong heterogeneities between adjacent cells within a layer, it would usually be preferable to select the linear interpolation scheme.

- *Maximum number of particles (NPMAX)*: Maximum number of particles available for particle tracking of advective transport in MOC3D. If it is set to zero, the model will calculate NPMAX according to equation 2.54.

$$NPMAX = 2 \cdot NPTPND \cdot NSROW \cdot NSCOL \cdot NSLAY \qquad (2.54)$$

where $NPTPND$ is the initial number of particles per cell (see below). The values $NSROW$, $NSCOL$, and $NSLAY$ are the number of rows, columns, and layers of the transport subgrid, respectively.

- *Courant number (CELDIS)* is the number of cells (or the fraction of a cell) that a particle may move through in one step (typically, 0.5 $\leq$ CELDIS $\leq$ 1.0).
- *Fraction limit for regenerating initial particles (FZERO)*: If the fraction of active cells having no particles exceeds FZERO, the program will automatically regenerate an initial particle distribution before continuing the simulation (typically, 0.01 $\leq$ FZERO $\leq$ 0.05).
- *Initial number of particles per cell (NPTPND)*: Valid options for default geometry of particle placement include 1, 2, 3, or 4 for one-dimensional transport simulation; 1, 4, 9, or 16 for two-dimensional transport simulation; and 1, 8, or 27 for three-dimensional transport simulation. The user can also customize initial placement of particles by specifying a negative number to NPTPND, pressing the Tab-key and entering local particle coordinates into table in the lower part of the dialog box shown in Fig. 2.64, where PNEWL, PNEWR and PNEWC are relative positions for the initial placement of particles in the layer, row and column direction, respectively. The local coordinate system range is from -0.5 to 0.5, and represents the relative distance within the cell about the node location at the center of the cell, so that the node is located at 0.0 in each direction.

2.6.5.4 MOC3D | Dispersion & Chemical Reaction

The types of reactions incorporated into MOC3D are restricted to those that can be represented by a first-order rate reaction, such as radioactive decay, or by a retardation factor, such as instantaneous, reversible, sorption-desorption reactions governed by a linear isotherm and constant distribution coefficient (K_d).

Use the Dispersion / Chemical Reaction (MOC3D) dialog box (Fig. 2.65) to specify the required data for each model layer as described below.

- *Simulate Dispersion*: Check this option, if dispersion should be included in the simulation.
- *First-order decay rate* λ [T^{-1}] typically represents radioactive decay of both the free and sorbed solute. A radioactive decay rate is usually expressed as a half-life ($t_{1/2}$). The half- life is the time required for the concentration to decrease to one-half of the original value. The decay rate λ is calculated by:

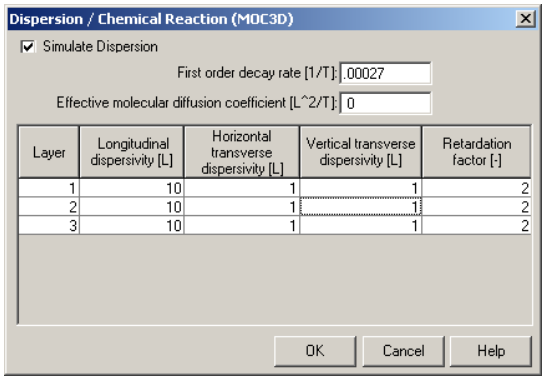


Fig. 2.65. The Dispersion / Chemical Reaction (MOC3D) dialog box

$$\lambda = \frac{\ln 2}{t_{1/2}} \tag{2.55}$$

- *Effective molecular diffusion coefficient* $[L^2T^{-1}]$ describes the diffusive flux of a solute in water from an area of greater concentration toward an area where it is less concentrated. Refer to Section 2.6.2.4 (page 94)for more about the molecular diffusion coefficient and dispersivity.
- *Longitudinal dispersivity* α_L $[L]$, *horizontal transverse dispersivity* α_{TH} $[L]$, and *vertical transverse dispersivity* α_{TV} $[L]$ describe the spreading of the solute concentration in groundwater caused by the irregular shape of the interconnected pore space and the velocity variations at the microscopic level as well as the unresolved macroscopic level. See Section 2.6.2.4 for details.
- *Retardation factor* R $[-]$: For a linear isotherm R is independent of the concentration field. R is calculated by

$$R = 1 + \frac{\rho_b}{n_e} \cdot K_d \tag{2.56}$$

where n_e is the effective porosity and rho_b is the bulk density of the porous medium.

2.6.5.5 MOC3D | Strong/Weak Flag

A flag is required for each cell within the transport subgrid. Where a fluid source is strong, new particles are added to replace old particles as they are advected out of that cell. Where a fluid sink is strong, particles are removed after they enter that cell and their effect has been accounted for. Where sources or sinks are weak, particles are neither added nor removed, and the source/sink effects are incorporated directly into appropriate changes in particle positions and concentrations. **A strong source or sink cell is indicated by the cell value of 1.**

2.6.5.6 MOC3D | Observation Wells

Cells of the transport subgrid can be designated as observation wells by assigning the value of 1 to the cells. At each observation well, the time, head, and concentration after each particle move will be written to the separate output file MOCOBS.OUT saved in the same folder as your model data. Note that this feature is to facilitate graphical post-processing of the calculated data using other software packages outside of **PM**.

2.6.5.7 MOC3D | Sink/Source Concentration

This menu is used for specifying the concentrations of point or distributed sources, including constant head cells, general-head boundary cells, rivers, wells and recharge cells. Except the concentrations associated with constant head cells, all source concentration values are specified in the Data Editor. If the concentration of a fluid source is not specified, the default value for the concentration is zero. The source concentration associated with the constant head cells are specified in the Source Concentration (Constant Head) dialog box (Fig. 2.66). The constant head cells are grouped into zones, which are defined by specifying unique negative values to the IBOUND array (see Section 2.4.3.1). Each zone has an associated source concentration value.

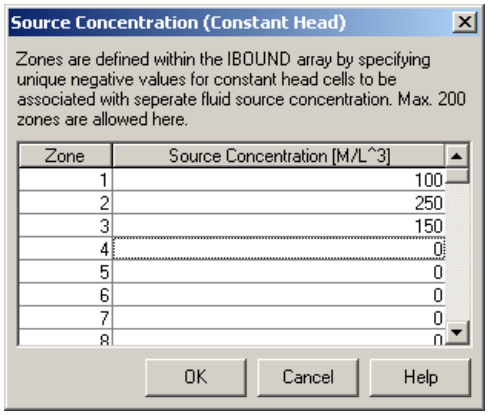


Fig. 2.66. The Source Concentration (Constant Head) dialog box

The concentration in the fluid leaving the aquifer at fluid sinks is assumed to have the same concentration as the fluid in the aquifer. However, if the fluid sink is associated with evaporation or transpiration, it is assumed that the fluid discharge mechanism will exclude dissolved chemicals, which results in an increase in concentration at the location of the sink.

Items of this menu are dimmed if the corresponding package in the *Models* | *MODFLOW* | *Flow Packages* menu are not used (checked). The specified concentration will be used by MOC3D if a corresponding menu item is checked. If a checked

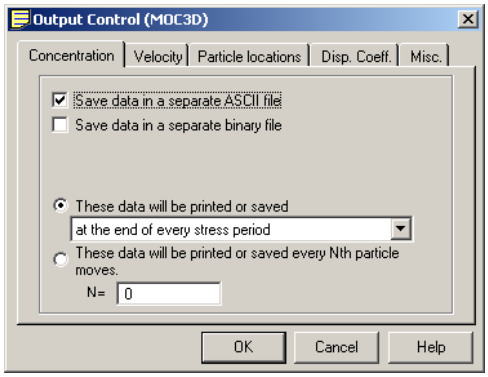


Fig. 2.67. The Output Control (MOC3D) dialog box

item is no longer necessary for a transport simulation, simply select the item again and deactivate it.

2.6.5.8 MOC3D | Output Control

The main output file of MOC3D is the listing file MOC3D.LST. MOC3D includes output options to create separate ASCII or binary files for concentration, velocity and the location of particles. Optionally the dispersion equation coefficients on cell faces can be written to the listing file. The dispersion equation coefficient is a combination of dispersion coefficient D, porosity n_e, thickness b and an appropriate grid dimension factor. For example, the dispersion equation coefficient for the interface between cells [k, j, i] and [k, j+1, i] in the column direction is $(n_e \cdot b \cdot D_{xx})_{k,j+1/2,i}/\Delta x$.

The output options for MOC3D are given in the Output Control (MOC3D) dialog box (Fig. 2.67). Most items in this dialog box are self-explanatory. The names of the separate ASCII or binary output files are given in Table 2.7.

Table 2.7 Names of the MOC3D output files

Output Term	**Filename**
Listing file	Path\MOC3D.lst
Concentration file (ASCII)	Path\mocconc.asc
Concentration file (binary)	Path\mocconc.bin
Velocity (ASCII)	Path\mocvel.asc
Velocity (binary)	Path\mocvel.bin
Particle location (ASCII)	Path\mocprt.asc
Particle location (binary)	Path\mocprt.bin

- Path is the folder in which the model is saved.

2.6.5.9 MOC3D | Concentration Observation

Select this menu item from the MOC3D menu to specify the locations of the concentration observation boreholes and their associated observed (measurement) data in a Concentration Observations dialog box. Its use is identical to the Head Observation dialog box (see Section 2.6.1.14). The only difference is that the head observations are replaced by concentration observations.

2.6.5.10 MOC3D | Run

Select this menu item to open the Run Moc3d dialog box (Fig. 2.68). The available settings of this dialog box are described below.

- The File Table has three columns:
  - *Generate*: Prior to running a flow simulation, **PM** uses the user-specified data to generate input files for MODFLOW and MOC3D. An input file will be generated if it does not exist or if the corresponding *Generate* box is checked. The user may click on a box to check or clear it. Normally, we do not need to worry about these boxes since **PM** will take care of the settings.
  - *Description* gives the names of the packages used in the model.
  - *Destination File* shows the paths and names of the input files of the model.
- Options:
  - *Regenerate all input files*: Check this option to force **PM** to generate all input files regardless the setting of the Generate boxes. This is useful if the input files have been deleted or overwritten by other programs.

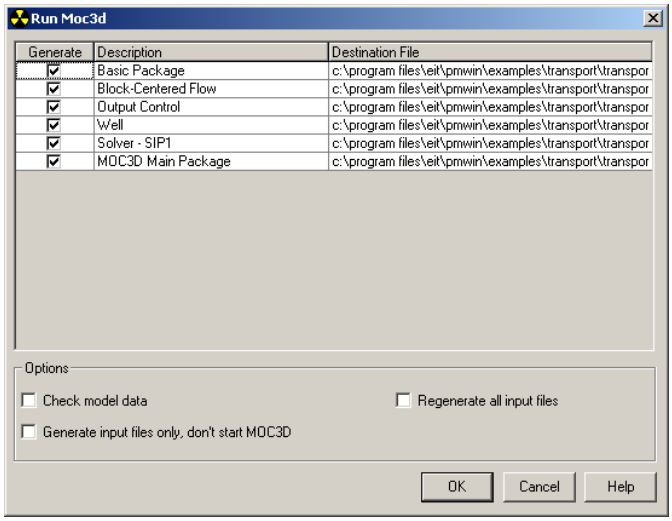


Fig. 2.68. The Run Moc3d dialog box

  - *Check the model data*: If this option is checked, **PM** will check the geometry of the model and the consistency of the model data as given in Table 2.6 before creating data files. The errors (if any) are saved in the file CHECK.LIS located in the same folder as the model data.
  - *Generate input files only, don't start MOC3D*: Check this option, if the user does not want to run MOC3D. The simulation can be started at a later time or can be started at the Command Prompt (DOS box) by executing the batch file MOC3D.BAT.
- *OK*: Click *OK* to generate MODFLOW and MOC3D input files. In addition to the input files, **PM** creates a batch file MOC3D.BAT in the model folder. When all files are generated, **PM** runs MOC3D.BAT in a Command Prompt-window (DOS box). During a simulation, MOC3D writes a detailed run record to the file MOC3D.LST saved in the model folder. MOC3D saves the simulation results in various unformatted (binary) files only if a transport simulation has been successfully completed. See the previous section for details about the output terms and the corresponding result files from MOC3D.

2.6.5.11 MOC3D | View

MOC3D | View | Run Listing File

Select this menu item to use the Text Viewer (see Section 2.3.4) to display the run list file MOC3D.LST, which contains a detailed run record saved by MOC3D.

MOC3D | View | Concentration Scatter Diagram

This menu item is available only if Concentration Observations have been defined (see Section 2.6.5.9). Select this menu item to open a Scatter Diagram (Concentration) dialog box, which is identical to the Scatter Diagram (Hydraulic Head) dialog box (Fig. 2.38), except the concentration values replace the head values.

MOC3D | View | Concentration-Time Curves

This menu item is available only if Concentration Observations have been defined (see Section 2.6.5.9). Select this menu item to open a Time Series Curves (Concentration) dialog box, which is identical to the Time Series Curves (Hydraulic Head) dialog box (Fig. 2.41), except the concentration values replace the head values.

2.6.6 MT3D

2.6.6.1 MT3D | Initial Concentration

MT3D requires the initial concentration of each active concentration cell, i.e. ICBUND > 0, at the beginning of a transport simulation. The values specified here are shared with MOC3D.

2.6.6.2 MT3D | Advection

The available settings of the Advection Package (MTADV1) dialog box (Fig. 2.69) are described below. Note that some of the simulation parameters are only required when a particular solution scheme is selected.

- *Solution Scheme*: MT3D provides four solution schemes for the advection term, including the method of characteristics (MOC), modified method of characteristics (MMOC), hybrid method of characteristics (HMOC),and upstream finite difference method.. Due to the problems of numerical dispersion and artificial oscillation, the upstream finite difference method is only suitable for solving transport problems not dominated by advection. When the grid Peclet number P_e ($P_e = \Delta x/\alpha L$; Δx is the grid spacing and αL is the longitudinal dispersivity) is smaller than two, the upstream finite difference method is reasonably accurate. It is advisable to use the upstream finite difference method anyway for obtaining first approximations in the initial stages of a modeling study.
  - The *method of characteristics (MOC)* scheme was implemented in the transport models MOC [73] and MOC3D (see Section 2.6.5.3), and has been widely used. One of the most desirable features of the MOC technique is that it is virtually free of numerical dispersion, which creates serious difficulty in many numerical schemes. The major drawback of the MOC scheme is that it can be slow and requires a large amount of computer memory when a large number of particles is required. Also, the computed concentrations sometimes tend to show artificial oscillations.
  - The *modified method of characteristics (MMOC)* uses one particle for each finite-difference cell and is normally faster than the MOC technique. At each new time level, a particle is placed at the nodal point of each finite-difference

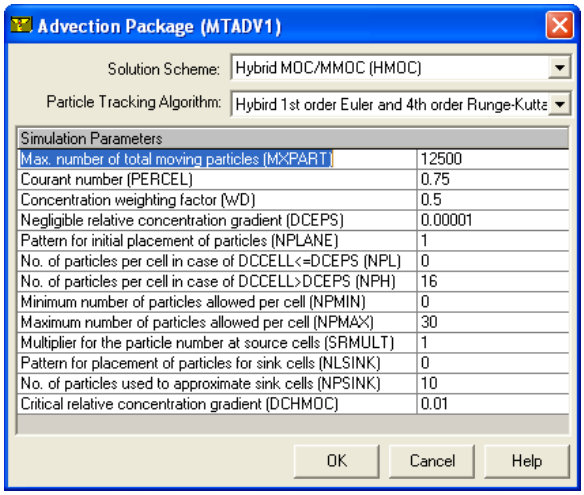


Fig. 2.69. The Advection Package (MTADV1) dialog box

cell. The particle is tracked backward to find its position at the old time level. The concentration associated with that position is used to approximate the advection-relevant average concentration at the cell, where the particle is placed. The MMOC technique is free of artificial oscillations if implemented with a lower-order velocity interpolation scheme (such as linear interpolation used in MT3D and MT3DMS). However, with a lower-order velocity interpolation scheme, the MMOC technique introduces some numerical dispersion, especially for sharp front problems.

  - The *hybrid method of characteristics (HMOC)* attempts to combine the strengths of the MOC and MMOC schemes by using an automatic adaptive scheme conceptually similar to the one proposed by Neumann [89]. The fundamental idea behind the scheme is automatic adaptation of the solution process to the nature of the concentration field. When sharp concentration fronts are present, the advection term is solved by MOC through the use of moving particles dynamically distributed around each front. Away from such fronts, the advection term is solved by MMOC. The criterion for controlling the switch between the MOC and MMOC schemes is given by DCHMOC (see below).

- *Particle Tracking Algorithm*: MT3D provides three particle tracking options: a first-order Euler algorithm, a fourth-order Runge-Kutta algorithm, and a combination of these two.
  - Using the first-order Euler algorithm, numerical errors tend to be large unless small transport steps are used. The allowed transport step t of a particle is determined by MT3D using equation 2.35 on page 91
  - The basic idea of the fourth-order Runge-Kutta method is to calculate the particle velocity four times for each tracking step: one at the initial point, twice at two trial midpoints, and once at a trial end point. A weighted velocity based on values evaluated at these four points is used to move the particle to a new position. The fourth-order Runge-Kutta method permits the use of larger tracking steps. However, the computational effort required by the fourth-order Runge-Kutta method is considerably larger than that required by the first-order Euler method. For this reason a mixed option combining both methods is introduced in MT3D.
  - The mixed option is implemented by automatic selection of the fourth-order Runge-Kutta algorithm for particles located in cells which contain or are adjacent to sinks or sources, and automatic selection of the first-order Euler algorithm for particles located elsewhere.
- *Maximum number of total moving particles (MXPART)* is the number of particles allowed in a simulation.
- *Courant number (PERCEL)* is the number of cells (or a fraction of a cell) any particle will be allowed to move in any direction in one transport step. Generally, $0.5 \leq \text{PERCEL} \leq 1$.
- *Concentration-weighting factor (WD)* lies between 0 and 1. The value of 0.5 is normally a good choice. This number can be adjusted to achieve better mass

balance. Generally, it can be increased toward 1 as advection becomes more dominant.

- *Negligible relative concentration gradient (DCEPS)* is a criterion for placing particles. A value around 10^{-5} is generally adequate. If DCEPS is greater than the relative cell concentration gradient $DCCELL_{k,i,j}$ (equation 2.36 on page 92), the higher number of particles NPH is placed in the cell [k, i, j], otherwise the lower number of particles NPL is placed (see NPH and NPL below)
- *Pattern for initial placement of particles (NPLANE)* is used to select a pattern for initial placement of moving particles.
  - NPLANE = 0, the random pattern is selected for initial placement. Particles are distributed randomly in both the horizontal and vertical directions (Fig. 2.48b on page 93). This option generally leads to smaller mass balance discrepancy in nonuniform or diverging/converging flow fields.
  - NPLANE > 0, the fixed pattern is selected for initial placement. The value of NPLANE serves as the number of "planes" on which initial particles are placed within each cell (Fig. 2.48a on page 93). This fixed pattern may work better than the random pattern only in relatively uniform flow fields. For two dimensional simulations in plan view, set NPLANE=1. For cross sectional or three dimensional simulations, NPLANE=2 is normally adequate. Increase NPLANE if more resolution in the vertical direction is desired.
- *No. of particles per cell in case of DCCELL $\leq$= DCEPS (NPL)* is the number of initial particles per cell to be placed at cells where the relative cell concentration gradient DCCELL is less than or equal to DCEPS. Generally, NPL can be set to zero since advection is considered insignificant under the condition DCCELL $\leq$ DCEPS. Setting NPL equal to NPH causes a uniform number of particles to be placed in every cell over the entire grid (i.e., the uniform approach).
- *No. of particles per cell in case of DCCELL $>$ DCEPS (NPH)* is the number of initial particles per cell to be placed at cells where the relative cell concentration gradient DCCELL is greater than DCEPS. The selection of NPH depends on the nature of the flow field and also the computer memory limitation. Generally, use a smaller number in relatively uniform flow fields and a larger number in relatively nonuniform flow fields. However, values exceeding 16 in two-dimensional simulations or 32 in three dimensional simulations are rarely necessary. If the random pattern is chosen, NPH particles are randomly distributed within the cell. If the fixed pattern is chosen, NPH is divided by NPLANE to yield the number of particles to be placed per plane, which is rounded to one of the values shown in Fig. 2.49 on page 94.
- *Minimum number of particles allowed per cell (NPMIN)*: If the number of particles in a cell at the end of a transport step is fewer than NPMIN, new particles are inserted into that cell to maintain a sufficient number of particles. NPMIN can be set to 0 in relatively uniform flow fields, and a number greater than zero in diverging/converging flow fields. Generally, a value between zero and four is adequate.

- *Maximum number of particles allowed per cell (NPMAX)*: If the number of particles in a cell exceeds NPMAX, particles are removed from that cell until NPMAX is met. Generally, NPMAX $\simeq 2 \times$ NPH.
- SRMULT is a multiplier for the particle number at source cells (SRMULT $\geq$ 1). In most cases, SRMULT = 1 is sufficient. However, better results may be obtained by increasing SRMULT.
- *Pattern for placement of particles for sink cells (NLSINK)* is used to select a pattern for initial placement of particles to approximate sink cells in the MMOC scheme. The convention is the same as that for NPLANE and it is generally adequate to set NLSINK equivalent to NPLANE.
- *Number of particles allowed to approximate sink cells (NPSINK)* is used in the MMOC scheme. The convention is the same as that for NPH and it is generally adequate to set NPSINK equivalent to NPLANE.
- *Critical relative concentration gradient (DCHMOC)* is used to select between MOC and MMOC in the HMOC solution scheme. MOC is selected at cells where DCCELL $>$ DCHMOC. MMOC is selected at cells where DCCELL $\leq$ DCHMOC.

2.6.6.3 MT3D | Dispersion

The use of this menu item is the same as *MT3DMS* | *Dispersion*, See Section 2.6.2.4 on page 94 for details.

2.6.6.4 MT3D | Chemical Reaction | Layer by Layer

Chemical reactions supported by MT3D include equilibrium-controlled sorption and first-order irreversible rate reactions, such as radioactive decay or biodegradation. It is generally assumed that equilibrium conditions exist between the aqueous-phase and solid-phase concentrations and that the sorption reaction is fast enough relative to groundwater velocity so that it can be treated as instantaneous. Consider using MT3DMS, if nonequilibrium (rate-limited) sorption needs to be simulated.

Use this menu item to open the Chemical Reaction Package (MTRCT1) dialog box (Fig. 2.70) to specify the required parameters on a layer-by-layer basis. The parameters are described below.

- *Type of sorption*: Sorption is implemented in MT3D through use of the retardation factor R. MT3D supports sorption types of *Linear isotherm (equilibrium) Freudlich isotherm (nonlinear, equilibrium)* and *Langmuir isotherm (nonlinear, equilibrium)*. See Section 2.6.2.6 for details.
- *Simulate the radioactive decay or biodegradation*: Check this box to simulate the effect of the first-order irreversible rate reactions. See the description of the reaction type *First-order irreversible reaction* on page 100 for details.

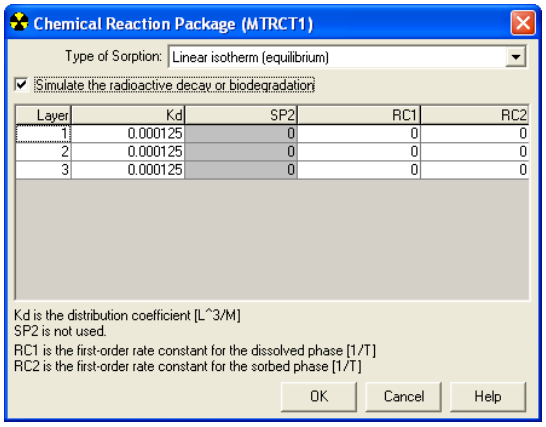


Fig. 2.70. The Chemical Reaction Package (MTRCT1) dialog box

2.6.6.5 MT3D | Chemical Reaction | Cell by Cell

Using the Data Editor, chemical reaction coefficients may be entered on a three dimensional cell by cell basis. This option provides the ability to have different reaction coefficients for different areas in a single model layer.

2.6.6.6 MT3D | Sink/Source Concentration

The use of this menu is the same as *MT3DMS/SEAWAT* | *Sink/Source Concentration*, except the use of the menu item *Time-Variant Specified Concentration*. A time variant specified concentration cell is defined by specifying the following data in the Data Editor. Note that Time Variant Specified Concentration may not be supported by some earlier version of MT3D.

- *Flag* [$-$]. A non zero value indicates that a cell is specified as a constant concentration cell. In a multiple stress period simulation, a constant-concentration cell, once defined, will remain a constant-concentration cell for the duration of the simulation, but its concentration value can be specified to vary in different stress periods. To change the concentration value in a particular stress period, simply set Flag to a non-zero value and assign the desired concentration value to Specified Concentration.
- *Specified Concentration* [ML^{-3}]. This value is the concentration in the cell at the beginning of a stress period.

2.6.6.7 MT3D | Concentration Observations

Select this menu item from the MT3D menu to specify the locations of the concentration observation boreholes and their associated observed (measurement) data in a Concentration Observations dialog box. Its use is identical to the Head Observation dialog box (see Section 2.6.1.14). The only difference is that the head observations are replaced by concentration observations.

2.6.6.8 MT3D | Output Control

Use the Output Control (MT3D/MT3DMS) dialog box (Fig. 2.71) to set the output options of MT3D. The options in this dialog box are grouped under three tabs described below.

- *Output Terms*: The MT3D transport model always generates a listing file OUTPUT.MT3, which documents the details of each simulation step. Optionally, you can save other output terms by checking the corresponding output terms in this tab. All output terms denoted by (ASCII) are also saved in the listing file. The calculated concentration values are saved in the unformatted binary file MT3D.UCN. In addition, MT3D96 can save the mass contained in each cell in the unformatted binary file MT3D.CBM. All output files are located in the same folder as your model. You can use the Result Extractor to read the unformatted binary files.
- *Output Times*: The value of the output frequency, NPRS, indicates whether the output is produced in terms of total elapsed simulation time or the transport step number. If NPRS$=0$, simulation results will only be saved at the end of simulation. If NPRS < 0, simulation results will be saved whenever the number of transport steps is an even multiple of NPRS. If NPRS > 0, simulation results will be saved at times as specified in the table shown in Fig. 2.72. There are two ways for specifying the output times. The user may click the table header Output Time and then enter a minimum time, a maximum time and a time interval between each output into an Output Time dialog box. **PM** will use these entries to calculate NPRS and the output times. The other way is to specify a positive NPRS and press the Tab key, then enter the output times into the table. Note that the output times are measured from the beginning of the simulation.
- *Misc.*:

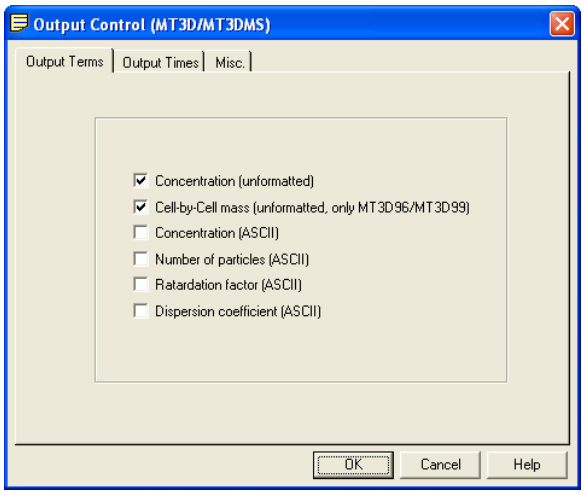


Fig. 2.71. The Output Control (MT3D/MT3DMS) dialog box

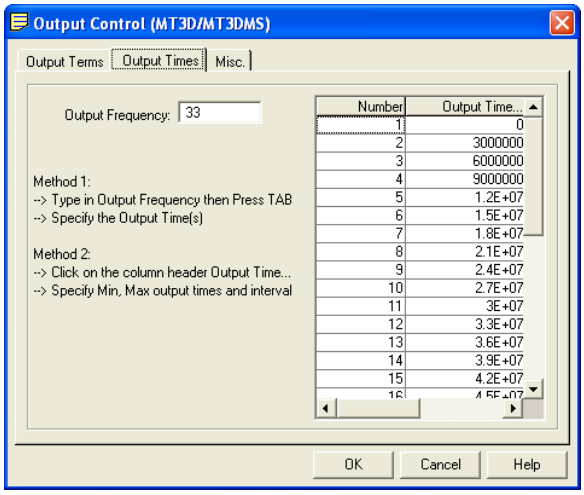


Fig. 2.72. The Output Times tab of the Output Control (MT3D/MT3DMS) dialog box

- *CINACT* is the predefined concentration value for an inactive concentration cell (ICBUND = 0). This value is a marker for these cells only and has no physical meaning.
- *THKMIN* is the minimum saturated thickness in a cell, expressed as the decimal fraction of the model layer thickness, below which the cell is considered inactive. THKMIN is only used by MT3D96 or later.
- *NPRMAS* indicates how frequently the mass budget information should be saved in the mass balance summary file MT3D.MAS.

2.6.6.9 MT3D | Run

The available settings of the Run MT3D/MT3D96 dialog box (Fig. 2.73) are described below.

- The File Table has three columns:
  - *Generate*: Prior to running a transport simulation, **PM** uses the user-specified data to generate input files for MT3D. An input file will be generated if it does not exist or if the corresponding *Generate* box is checked. The user may click on a box to check or clear it. Normally, we do not need to worry about these boxes since **PM** will take care of the settings.
  - *Description* gives the names of the packages used in the model.
  - *Destination File* shows the paths and names of the input files of the model.
- Options:
  - *Regenerate all input files*: Check this option to force **PM** to generate all input files regardless the setting of the Generate boxes. This is useful if the input files have been deleted or overwritten by other programs.

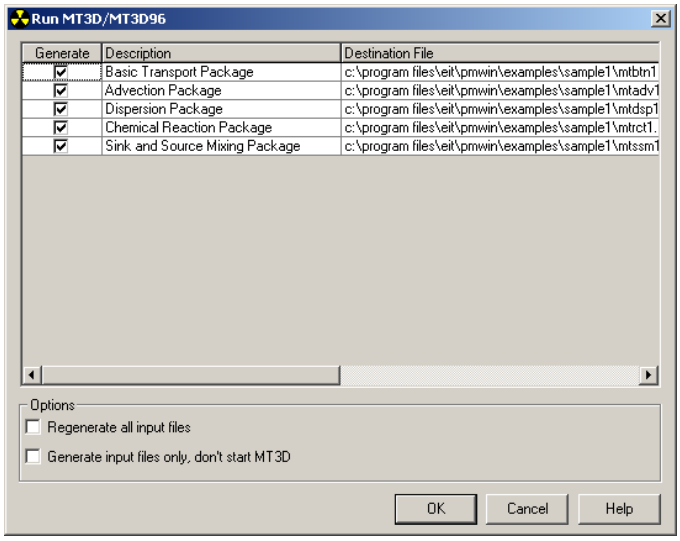


Fig. 2.73. The Run MT3D/MT3D96 dialog box

  - *Generate input files only, don't start MT3D*: Check this option, if the user does not want to run MT3D. The simulation can be started at a later time or can be started at the Command Prompt (DOS box) by executing the batch file MT3D.BAT.
- *OK*: Click *OK* to generate MT3D input files. In addition to the input files, **PM** creates a batch file MT3D.BAT saved in the model folder. When all files are generated, **PM** automatically runs MT3D.BAT in a Command Prompt-window (DOS box). During a simulation, MT3D writes a detailed run record to the file OUTPUT.MT3 saved in the model folder. See the previous section for details about the output terms.

2.6.6.10 MT3D | View

MT3D | View | Run Listing File

Select this menu item to use the Text Viewer (see Section 2.3.4) to display the run list file OUTPUT.MT3, which contains a detailed run record saved by MT3D.

MT3D | View | Concentration Scatter Diagram

This menu item is available only if Concentration Observations have been defined (see Section 2.6.6.7 on page 131). Select this menu item to open a Scatter Diagram (Concentration) dialog box, which is identical to the Scatter Diagram (Hydraulic Head) dialog box (Fig. 2.38 on page 78), except the concentration values replace the head values.

MT3D | View | Concentration-Time Curves

This menu item is available only if Concentration Observations have been defined (see Section 2.6.6.7 on page 131). Select this menu item to open a Time Series Curves (Concentration) dialog box, which is identical to the Time Series Curves (Hydraulic Head) dialog box (Fig. 2.41 on page 82), except the concentration values replace the head values.

2.6.7 MODFLOW-2000 (Parameter Estimation)

This section describes the interface for the built-in parameter estimation capability of MODFLOW-2000. The parameters and/or excitations, which can be estimated by MODFLOW-2000, are listed in Table 2.8. Since the BCF package does not support parameterization of aquifer parameters, it cannot be used with the parameter estimation procedures of MODFLOW-2000. In other words, if the user plans to use MODFLOW-2000 to estimate aquifer parameters, then one has to use the LPF package with adjustable aquifer parameters HK, VK, HANI, VANI. Ss and Sy. See Section 2.3.4 for how to switch between the BCF and LPF packages.

During a parameter estimation process, MODFLOW-2000 searches optimum parameter values for which the sum of squared deviations between model-calculated and observed hydraulic heads at the observation boreholes is reduced to a minimum. The coordinates of the observation boreholes and observed head values are given in *MODFLOW-2000 (Parameter Estimation) | Head Observations*. It is to note that MODFLOW-2000 does not accept drawdown observations; rather it has an option of using the temporal changes in hydraulic heads as observations, see Section 2.6.1.14 for details. Of particular note is that a simultaneous fit of highly correlated parameters, for example HK and recharge values on the basis of observed heads only, is of little value in steady-state problems due to the non-uniqueness of such a fit. In those cases, the ability of using prior information and flow observation data in MODFLOW-2000 could help in solving problems.
The parameters to be estimated are defined in the following steps.

Table 2.8 Adjustable parameters through MODFLOW-2000 within **PM**

Packages	Abbreviation	Adjustable Parameters
Block-Centered Flow	BCF	No aquifer parameters can be estimated.
Layer-Property Flow	LPF	All layer types: HK, HANI, VANI, VK, Ss, and Sy
Drain	DRN	Conductance of drain cells
Evapotranspiration	EVT	Maximum evapotranspiration rate
General-Head Boundary	GHB	Conductance of GHB cells
Horizontal Flow Barrier	HFB6	Hydraulic characteristic of barrier
Recharge	RCH	Recharge flux
River	RIV	Conductance of RIV cells
Stream-Flow Routine	STR	Conductance of STR cells
Well	WEL	Pumping or injection rates of WEL cells

► To define an adjustable parameter for estimation

1. Select a parameter or a package from the *Parameters* or *Models* | *MODFLOW* | *Flow Packages* menus, for example Horizontal Hydraulic Conductivity, Recharge, or Well.
2. Assign a parameter number and initial (guessed) parameter values to the cells, where the parameter values should be estimated. The parameter number needs to be unique within a parameter type (e.g., HK or Ss) and may be any integer ranging between 1 and 500. Set the parameter number to zero, if the specified parameter value should not be estimated. Please note the following rules when assigning parameter values and parameter numbers:
   - During a parameter estimation process, the parameter values for an estimation-iteration are calculated as the product of the parameter's initial cell-values and a parameter multiplier (PARVAL). The latter is to be estimated by MODFLOW-2000. It is to note that if the parameter's initial cell-values are heterogeneously distributed, then the result is also a distribution scaled by the estimated parameter multiplier. In contrast, if the value of 1 is used as the parameter's initial cell-value, then the estimated parameter multiplier represents the physical parameter value.
   - To estimate the conductance values of head-dependent cells (e.g., drain, general head-boundary, river or stream cells) or pumping rates of wells, a non-zero conductance value or pumping rate must be assigned to those cells. Conductance values or pumping rate will not be adjusted, if the user-specified values are equal to zero.
   - In a transient flow model, when a parameter is varying with time, parameter numbers should not be repeated in different stress periods. That is, different parameter numbers should be used for different stress periods.
3. Select *MODFLOW-2000 (Parameter Estimation)* | *Parameter List* to open a List of Parameters (MODFLOW-2000) dialog box, which lists all parameters defined in previous steps and provides an overview of all parameters. The dialog box also allows selecting or un-selecting parameters for estimation (see Section 2.6.7.1).

2.6.7.1 MODFLOW-2000 (Parameter Estimation) | Simulation Settings

The required parameters and execution options for MODFLOW-2000 are specified in the List of Parameters (MODFLOW-2000) dialog box (Fig. 2.74). The available settings are grouped under four tabs described below. Using the Save button, the user can save the settings in separate ASCII files, which can be loaded at a later time by using the Load button. Click the Update button to retrieve the estimated parameter values, saved in the MF2KOUT._B file. The Update button is disabled and dimmed, if this file is not available.

The Parameters Tab

The Parameters Tab contains a table that gives an overview of the initial values and properties of estimated parameters. The initial value (PARVAL) of parameter is the

arithmetical mean of the cell values of that parameter. The parameter's lower bound PARLBND and upper bound PARUBND default to two orders lower andhigher than PARVAL, respectively.

If a parameter is removed by changing the parameter number to zero in the Data Editor, the corresponding parameter in the table is ignored. **PM** does not delete that adjustable parameter from the table. To delete the parameter, click on its record selector (before the first column of the table), then press the *Del* key. Note that the user cannot manually add a parameter to the table. If a parameter is deleted by mistake, simply click the Cancel button to discard all changes, or click the OK button to accept changes, and then open the Simulation Settings (MODFLOW-2000) dialog box again to recover the "lost" parameter.

The meaning of each column of the table is described below. By clicking on a column header, the parameters can be sorted in ascending order using the values of that column.

- *PARNAM*: While editing data of a certain aquifer parameter or flow package, the spatial extent of an estimated parameter is defined by assigning a parameter number to the cells of interest. **PM** automatically assigns a PARNAM by combining that parameter number with the short names of the aquifer parameter (i.e., HK, VK, VANI, HANI, SS and SY), or package. For example, if parameter numbers 1 and 2 are specified for the Recharge package, then RCH_1 and RCH_2 are assigned to PARNAM (Fig. 2.74). Modification of the assigned names is not allowed.
- *Active*: The value of an estimated parameter will only be adjusted if Active is checked. Otherwise the user-specified cell values will be used for the simulation.

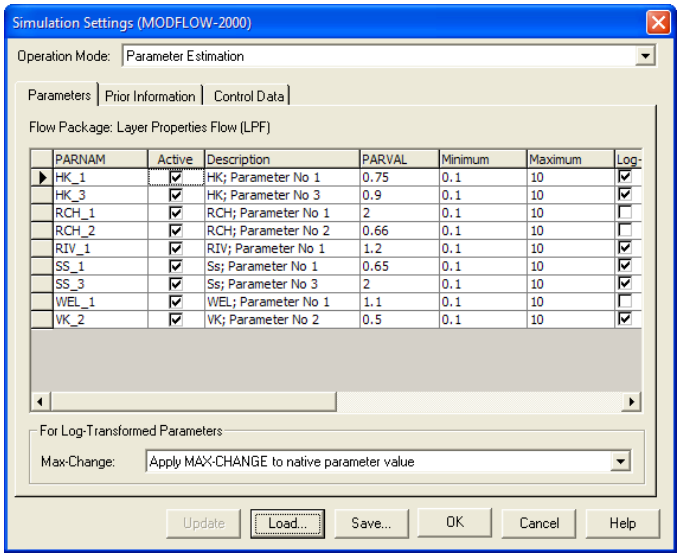


Fig. 2.74. The Simulation Settings (MODFLOW-2000) dialog box

When switching from the BCF to LPF (or from LPF to BCF) package, some aquifer parameters might become unadjustable (e.g., T, S are not adjustable when using the LPF package), and they will be indicated by gray background color. Normally, the total number of active parameters should not exceed 10, although **PM** allows 500 parameters.

- *Description*: A text describing the parameter can be entered here (optional), for example, "recharge zone one". A maximum of 120 characters is allowed.
- *PARVAL* is the initial parameter multiplier for PARNAM.
- *Minimum* and *Maximum* are the reasonable minimum and maximum scaling factors for the parameter. These values are used solely to determine how the final optimized value of this parameter compares to a reasonable range of values. For log-transformed parameters, untransformed values should be used.
- *Log-transform*: Check this flag to log-transform the parameter. Typically log-trans-formed parameters are those for which negative values are not reasonable (for example hydraulic conductivity).

The Prior Information Tab

It often happens that we have some information concerning the parameters that we wish to optimize, and that we obtained this information independently of the current experiment. This information may be in the form of other unrelated estimates of some or all of the parameters, or of relationships between parameters. It is often useful to include this information in the parameter estimation process because it may lend stability to the process.

To define prior information, first check the Active box in the Prior Information tab, and then enter the prior information equation in the Prior Information column. The syntax of a prior information line is

$$\begin{aligned} &Eqnam\ \ Prm\ =\ [Sign]\ \ [Coef\,*]\ \ Pnam\ \ [Sign\ \ [Coef*]\ \ Pnam\ \ [Sign...]] \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad STAT\ \ Statp\ \ Stat\text{-}flag\ \ Plot\text{-}Symbol \end{aligned} \tag{2.57}$$

All components of equation 2.57 must be separated by one space. Following Hill and others [63], the components are defined below:

- *Eqnam* is a user-supplied name (up to 10 nonblank characters) for a prior-information equation.
- *Prm* is the prior estimate for prior-information equation Eqnam. Prm always needs to be specified as a native, untransformed value. That is even if the parameter is specified as being log-transformed (see the Parameters tab above), Prm needs to be the untransformed value.
- = indicates the equal sign.
- *Sign* is either + or -. The [Sign] after = is optional and is assumed to be + unless otherwise specified.
- *Coef* is the multiplication coefficient for the parameter following the * in the prior-information equation. Coef can be specified with or without a decimal point and can be specified in scientific notation (e.g., 3.123E+03).

- * indicates multiplication.
- *Pnam* is the parameter name. For aquifer parameters (i.e., HK, VK, HANI, VANI, SS and SY) Pnam is the same as PARNAM given in the Parameters tab (see above). For time-varying parameters (e.g., RCH, WEL...), Pnam is a combination of PARNAM and the stress period number, to which Pnam pertains. For example, for parameter number 2 of recharge (RCH_2) in the stress period 3, Pnam = RCH_2_3.
  If the parameter is designated as being log-transformed, the prior-information equation may contain only one parameter name.
- *STAT* must be entered literally.
- *Statp* is the value from which the weight for prior-information equation Eqnam is calculated, as determined using Stat-flag.
- *Stat-flag* is a flag identifying how the weight for prior-information equation Eqnam is to be calculated. This depends both on whether the user chooses to specify the variance, standard deviation, or coefficient of variation, and whether, for log-transformed parameters, the user chooses to specify the statistic related to the native, untransformed parameter, or to the transformed parameter.
  1. Stat-flag = 0: Statp is the variance associated with Prm, and is related to the native prior value. $Weight = 1/Statp$ unless the parameter is defined as log-transformed, in which case equation 27 of Hill and others [63] is used to convert Statp (which equals σ_b^2 of equation 27) to $\sigma_{\ln b}^2$, and $Weight = 1/\sigma_{\ln b}^2$.
  2. Stat-flag = 1: Statp is the standard deviation associated with Prm, and is related to the native prior value. $Weight = 1/Statp^2$ unless the parameter is defined as log-transformed, in which case equation 27 of Hill and others [63] is used to convert Statp (which equals σ_b of equation 27) to $\sigma_{\ln b}^2$, and $Weight = 1/\sigma_{\ln b}^2$.
  3. Stat-flag = 2: Statp is the coefficient of variation associated with Prm, and is related to the native prior value. $Weight = 1/(Statp \times Prm)^2$ unless the parameter is defined as log-transformed, in which case equation 27 of Hill and others [63] is used to convert Statp (which equals σ_b/b of equation 27) to $\sigma_{\ln b}^2$, and $Weight = 1/\sigma_{\ln b}^2$.
  4. Stat-flag = 10: Statp is the variance associated with the log (base 10) transform of Prm. $Weight = 1/(Statp \times 2.3026^2)$.
  5. Stat-flag = 11: Statp is the standard deviation associated with the log (base 10) transform of Prm. $Weight = 1/(Statp^2 \times 2.3026^2)$.
  6. Stat-flag = 12: Statp is the coefficient of variation associated with the log (base 10) transform of Prm. $Weight = 1/[(Statp \times \log_{10}(PRM))^2 \times 2.3026^2]$.
- *Plot-Symbol* is an integer that will be written to output files intended for graphical analysis to allow control of the symbols used when plotting data related to the prior information.

The following lines show some examples, refer to Hill ([62], p. 43ff) and Hill and others ([63], p. 83ff) for more details about the use of the prior information.

```
PRCH1 22 = 36500 * RCH_1_1 STAT 5.0 1 4
PHK1 10 = HK_1 STAT 0.5 11 5
PS1&2 0.02 = 20 * SS_1 + 30 * SS_2 STAT 0.5 11 5
```

The Control Data Tab

The control data are used to control the regression calculations. The control data are written in the input file (PES.DAT) for the Parameter Estimation Process. Following Hill and others [63] the items of the control data are described below.

- *MAX-ITER* is the maximum number of parameter-estimation iterations. If MAX-ITER = 0, the program calculates the variance-covariance matrix on parameters and related statistics (the parameter correlation coefficients generally are of most interest) using the starting parameter values, and parameter estimation stops after one-iteration. Note that the starting parameter values are obtained by multiplying PARVAL with the cell-values of the parameter, see Parameters Tab.
- *MAX-CHANGE* is the maximum fractional change for parameter values in one iteration step. MAX-CHANGE commonly equals to 2.0, or less if parameter values are unstable during parameter-estimation iterations.
- *TOL* is the parameter-estimation closure criterion, as a fractional change in parameter values. TOL commonly equals 0.01. Larger values often are used during preliminary calibration processes; value as small as 0.001 may be used for theoretical works.
- *SOSC* is the second convergence criterion discussed in Hill ([62], p.12). If SOSC $\neq$ 0.0, parameter estimation will converge if the least-squares objective function does not decrease more than SOSC $\times$ 100 percent over two parameter-estimation iterations. SOSC usually equals 0.0. Typical nonzero values of SOSC are 0.01 and 0.05.
- *RMAR* is used along with RMARM to calculate the Marquardt parameter, which is used to improve regression performance for ill-posed problems (Theil [111]; Seber and Wild [107]). Initially the Marquardt parameter is set to zero for each parameter-estimation iteration. For iterations in which the parameter changes are unlikely to reduce the value of the objective function, the Marquardt parameter is increased according to $m_r^{new} = RMARM \times m_r^{old} + RMAR$ until the condition is no longer met or until m_r^{new} is greater than 1. Typically, RMAR = 0.001.
- *RMARM* is the Marquardt parameter multiplier, which is used along with RMAR to determine the Marquardt parameter (see above).
- *CSA* is the search-direction adjustment parameter used in the Marquardt procedure. Usually equals 0.08.
- *FCONV* is a flag and a value used to allow coarser solver convergence criteria for early parameter-estimation iterations. If FCONV equals zero, coarser convergence criteria are not used. Commonly, FCONV = 0.0. Typical non-zero values would be 5.0 or 1.0, and these can produce much smaller execution times in some circumstances.

The Options Tab

Two options are available:

- *Run Mode*:
  - *Perform Parameter Estimation* is the default run mode, which instructs MOD-FLOW-2000 to estimate values of active parameters listed in the Parameters tab.
  - *Perform Sensitivity Analysis* directs MODFLOW-2000 to evaluate sensitivities using the initial PARVAL and parameter values. Using this option, MODFLOW-2000 calculates one-percent sensitivities for hydraulic heads for the entire grid. The one-percent sensitivities can be contoured just like hydraulic heads can be countered. The one-percent scaled sensitivity map can be used to identify where additional observations of hydraulic head would be most important to the estimation of different parameters and to compare the sensitivity of hydraulic heads throughout the model to different parameters.
  - *Perform Forward Model Run using PARVAL values given in the Parameters tab*: This option directs MODFLOW-2000 to replace the model parameters by the product of PARVAL values and the cell-values of parameters, and then perform a forward model run.
- *Max-Change*: This option determines whether MAX-CHANGE specified in the Control Data tab is applied to the native parameter value or to the log transform of the parameter value. This option only applies to log-transformed parameters.

2.6.7.2 MODFLOW-2000 (Parameter Estimation) | Head Observations

Select *Head Observations* from the *MODFLOW-2000 (Parameter Estimation)* menu (or *MODFLOW* or *PEST* menus) to specify the locations of the head observation boreholes and their associated observed (measurement) data in a Head Observation dialog box (see Section 2.6.1.14 on page 70 for details).

When this menu item is selected (and checked), the Head Observation package of MODFLOW-2000 will use the head observation data for the parameter estimation. If you do not want to use the Head Observation package (and the head observation data), select the menu item again and click the Deactivate button.

2.6.7.3 MODFLOW-2000 (Parameter Estimation) | Flow Observations

This menu is used for specifying the flow observation data associated with drain, general head boundary, river or constant head boundary cells. Each sub-menu is enabled only if the corresponding flow package is in use. When a sub-menu is selected (and checked), its flow observation data will be used for the parameter estimation. If the user does not want to use the flow observation data, select the sub-menu again and click the Deactivate button.

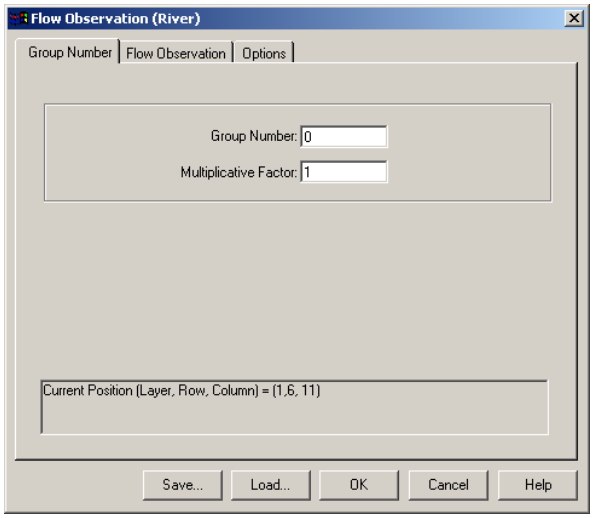


Fig. 2.75. The Flow Observation (River) dialog box

Flow observations are defined by assigning parameters to model cells using the Flow Observation dialog box (Fig. 2.75) of the Data Editor. The dialog box consists of two tabs as described below.

The Group Number Tab

A flow observation is commonly represented by a group of cells with the same Group Number. For each cell group, MODFLOW-2000 compares the simulated flow rate (gain or loss) with the observation data specified in the Flow Observation tab. The simulated flow rate of a cell group y' $[L^3T^{-1}]$ is calculated by

$$y' = \sum_{n=1}^{nqcl} f_n \cdot q_n \tag{2.58}$$

where $nqcl$ is the number of cells in the cell group; f_n is a user-specified multiplicative factor; q_n [L3T-1] is the simulated flow rate at one cell. Generally f_n = 1.0. However, if a gauging site is located within a cell instead of at the edge of the cell, f_n needs to be less than 1.0 so that only part of the simulated flow for the cell is included in y'.

The Flow Observation Tab

The Flow Observation tab (Fig. 2.76) is used to specify the names of cell groups and their associated observed (measurement) data. The options of this tab are described below.

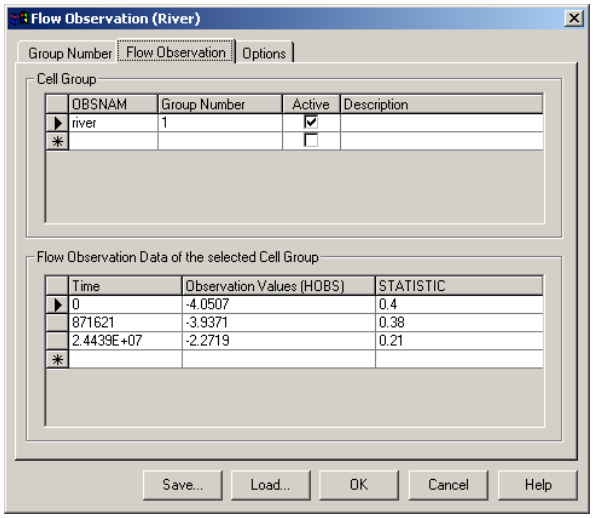


Fig. 2.76. The Flow Observation tab of the Flow Observation (River) dialog box

1. *Cell Group*: Each row of the table pertains to a group of cells. The name (OBSNAM) and the associated group number (Group Number) of each cell group are to be specified in the table. A cell group is active if the Active flag is checked. To add a cell group, scroll down to the end of the table and simply type the name and group number to the last (blank) row. To delete a cell group, the user selects the row to be deleted by clicking on its record selector (▭ before the first column of the table), then pressing the *Del* key.
   After a simulation, the user may select *View* | *Scatter Diagram* from the *MODFLOW-2000 (Parameter Estimation)* menu to compare the observed and calculated values. The user may also select *View* | *Time Series Curves* from the same menu to display time-series curves of both the calculated and observed values.
2. *Flow Observation Data* of the selected Cell Group contains the data pertained to the cell group marked by ▶ on the Cell Group table. Inserting or deleting an observation (row) is identical to the Cell Group table.
   a) *Time*: The observation time, to which the measurement pertains, is measured from the beginning of the model simulation. The user may specify the observation times in any order. By clicking on the column header or the OK button, the observation times (and the associated values) will be sorted in ascending order.
   b) *Observation values (HOBS)* contain the flow rates observed at the observation times. Negative values should be assigned when water leaves the groundwater system.
   c) *Statistic*: MODFLOW-2000 reads statistics from which the weights are calculated. The physical meaning of Statistic is controlled by the Option tab (see below).

The Options Tab

The Statistic Option defines the physical meaning of Statistic specified in the Flow Observation tab. It also defines how the weights are calculated. Refer to Hill [62] for more details about the role of statistics and weights in solving regression problems.

2.6.7.4 MODFLOW-2000 (Parameter Estimation) | Run

MODFLOW-2000

Select this menu item to start MODFLOW-2000. The available settings of the Run MODFLOW-2000 (Sensitivity Analysis/Parameter Estimation) dialog box (Fig. 2.77) are described below.

- The File Table has three columns:
  - *Generate*: Prior to running the program, **PM** uses the user-specified data to generate input files for MODFLOW-2000. An input file will be generated if it does not exist or if the corresponding *Generate* box is checked. The user may click on a box to check or clear it. Normally, we do not need to worry about these boxes since **PM** will take care of the settings.
  - *Description* gives the names of the packages used in the model.
  - *Destination File* shows the paths and names of the input files of the model.
- Options:

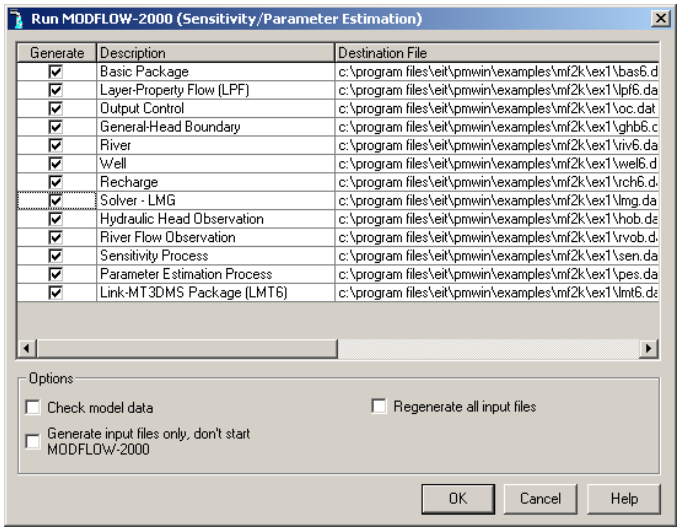


Fig. 2.77. The Run MODFLOW-2000 (Sensitivity Analysis/Parameter Estimation) dialog box

  - *Regenerate all input files*: Check this option to force **PM** to generate all input files regardless the setting of the Generate boxes. This is useful if the input files have been deleted or overwritten by other programs.
  - *Generate input files only, don't start MODFLOW-2000*: Check this option, if the user does not want to run MODFLOW-2000. The simulation can be started at a later time or can be started at the Command Prompt (DOS box) by executing the batch file MF2K.BAT.
  - *Check the model data*: If this option is checked, **PM** will check the geometry of the model and the consistency of the model data as given in Table 2.6 (page 77) before creating data files. The errors (if any) are saved in the file CHECK.LIS located in the same folder as the model data.
- *OK*: Click *OK* to generate MODFLOW-2000 input files. In addition to the input files, **PM** creates a batch file MF2K.BAT in the model folder. When all files are generated, **PM** automatically runs MF2K.BAT in a Command Prompt-window (DOS box). During the parameter estimation process, the user will notice that the parameter names (PARNAM) of time-varying parameters (e.g., RCH, WEL) are further combined with the stress period number, to which the parameter pertains. For example, parameter number 2 of recharge in stress period 3 is indicated by RCH_2_3. For steady state simulations, the string "_1" is used.
  After completing the parameter estimation process, MODFLOW-2000 prints the optimized parameter values to the file MF2KOUT._b in the model folder. The model results after the parameter estimation process are calculated by using the optimized parameter values. During a parameter estimation process, MODFLOW-2000 does not modify the original model data. This provides a greater security for the model data, because a parameter estimation process does not necessarily lead to a success.

PEST-ASP+MODFLOW-2000

Select this menu item to start parameter estimation with the coupled approach PEST-ASP + MODFLOW-2000. In this case, the derivatives of model outputs with respect to adjustable parameters are calculated by MODFLOW-ASP[35](a modified version of MODFLOW-2000) and the parameter estimation is done by PEST-ASP. This approach combines the strengths of both programs. The available settings of the Run PEST-ASP + MODFLOW-2000 dialog box (Fig. 2.78) are described below.

- The File Table has three columns:
  - *Generate*: Prior to running the program, **PM** uses the user-specified data to generate input files for MODFLOW-ASP and PEST-ASP. An input file will be generated only if the corresponding Generate box is checked. The user may click on a box to check or clear it. Normally, we do not need to worry about these boxes since **PM** will take care of the settings.
  - *Description* gives the names of the packages used in the model.
  - *Destination File* shows the paths and names of the input files of the model.
- Options:

- *Regenerate all input files*: Check this option to force **PM** to generate all input files regardless the setting of the Generate boxes. This is useful if the input files have been deleted or overwritten by other programs.
- *Generate input files only, don't start PEST-ASP*: Check this option, if the user does not want to run PEST-ASP + MODFLOW-2000. The simulation can be started at a later time or can be started at the Command Prompt (DOS box) by executing the batch file PESTMF2K.BAT.
- *Check the model data*: If this option is checked, **PM** will check the geometry of the model and the consistency of the model data as given in Table 2.6 (page 77) before creating data files. The errors (if any) are saved in the file CHECK.LIS located in the same folder as the model data.
- *Let PEST-ASP calculate Derivatives*: Although the derivatives calculated by MODFLOW-ASP using the sensitivity equation method is more accurate, sometimes the slight loss of numerical precision incurred through the use of derivatives calculated by PEST-ASP using the perturbation (finite-difference) method appears to abet, rather than hinder, the parameter estimation process. This option should be tried if a parameter estimation process fails to converge.

- *OK*: Click OK to generate the input files. In addition, **PM** creates a batch files PESTMF2K.BAT in the model folder. When all files are generated, **PM** automatically runs PESTMF2K in a Command Prompt-window (DOS box). After completing the parameter estimation process, PEST-ASP + MODFLOW-2000 prints the optimized parameter values to the file MF2KOUT._B in the model folder. The model results after the parameter estimation process are calculated by using the optimized parameter values. During a parameter estimation process, PEST-ASP

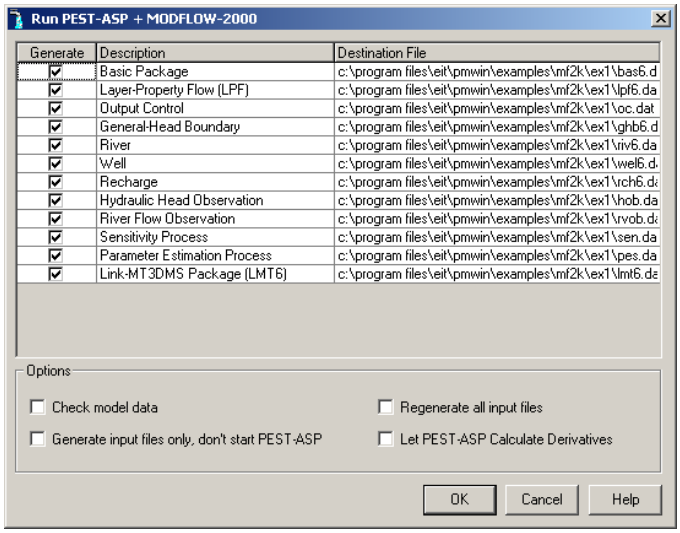


Fig. 2.78. The Run PEST-ASP + MODFLOW-2000 dialog box

+ MODFLOW-2000 does not modify the original model data. This provides a greater security to the model data, because a parameter estimation process does not necessarily lead to a success.

2.6.7.5 MODFLOW-2000 (Parameter Estimation) | View

MODFLOW-2000 (Parameter Estimation) | View | Global Listing File

Select this menu item to use the Text Viewer (see Section 2.3.4) to display the global listing file MF2K.GLOBAL_LISTING, which contains the parameter values and statistics for parameter-estimation iterations, the optimized value of each adjustable parameter together with that parameter's 95% confidence interval. It tabulates the set of field measurements, their optimized model-calculated counterparts, the difference between each pair, and certain functions of these differences.

MODFLOW-2000 (Parameter Estimation) | View | Forward Run Listing File

During a parameter estimation process, forward runs are repeated and the run record is saved in the listing file OUTPUT.DAT. Listing files are overwritten during subsequent forward model runs and thus only the listing file unique to final parameter values is available for inspection with the Text Viewer (see Section 2.3.4).

Parameter estimation processes are often terminated unexpectedly because the groundwater flow process of MODFLOW-2000 fails to complete a flow calculation due to an unsuitable parameter combination used by an estimation-iteration. In that case, MODFLOW-2000 writes error messages to the OUTPUT.DAT file and terminates the simulation. It is therefore recommended to check this file when MODFLOW-2000 fails to complete the parameter estimation iterations.

MODFLOW-2000 (Parameter Estimation) | View | Estimated Parameter Values

At the end of each optimization-iteration MODFLOW-2000 writes the estimated parameter set to a file named MF2KOUT._B. Select this menu item to use the Text Viewer (see Section 2.3.4) to display this file. The estimated parameter values are displayed using the parameter name PARNAM given in the Parameters tab of the List of Parameters (MODFLOW-2000) dialog box (Fig. 2.74). The parameter names (PARNAM) of time-varying parameters (e.g., RCH, WEL...) are combined with the stress period number, to which the parameter pertains. For example, parameter number 2 of recharge in stress period 3 is indicated by RCH_2_3. For steady state simulations, the string "_1" is used as the stress period number.

Using values from intermediate parameter-estimation iterations, that are likely to be closer to the optimal parameter values, often reduces execution time.

MODFLOW-2000 (Parameter Estimation) | View | Dimensionless Scaled Sensitivities

Select this menu item to use the Text Viewer (see Section 2.3.4 for linking a Text Viewer with **PM**) to display the file MF2KOUT._SD, which contains dimensionless scaled sensitivity values that can be used to compare the importance of different observations to the estimation of a single parameter or the importance of different parameters to the calculation of a simulated value (Hill [62]).

MODFLOW-2000 (Parameter Estimation) | View | Composite Scaled Sensitivities

Select this menu item to use the Text Viewer (see Section 2.3.4 for linking a Text Viewer with **PM**) to display the file MF2KOUT._SC, which contains composite scaled sensitivity values that indicate the total amount of information provided by the observations for the estimation of one parameter. If some parameters have composite scaled sensitivities that are less than about 0.01 times the largest composite scaled sensitivity, it is likely that the regression will have trouble converging (Hill [62]). A parameter with large composite scaled sensitivity and many large dimensionless scaled sensitivities is probably more reliably estimated than a parameter with a large composite scaled sensitivity and one large dimensionless scaled sensitivity because the error of the single important observation is propagated directly into the estimate (Hill [63]).

MODFLOW-2000 (Parameter Estimation) | View | One-Percent Scaled Sensitivities

Select this menu item to use the Text Viewer (see Section 2.3.4 for linking a Text Viewer with **PM**) to display the file MF2KOUT._S1, which contains one-percent scaled sensitivity values that indicate an approximate amount of information provided by the observations for the estimation of one parameter.

MODFLOW-2000 (Parameter Estimation) | View | One-Percent Scaled Sensitivities Arrays

The one-percent sensitivities for hydraulic heads are calculated for the entire grid and can be contoured just like hydraulic heads can be contoured. The one-percent scaled sensitivity map can be used to identify where additional observations of hydraulic head would be most important to the estimation of different parameters and to compare the sensitivity of hydraulic heads throughout the model to different parameters ([62]).

MODFLOW-2000 (Parameter Estimation) | View | Scatter Diagram

This menu item is available only if head observations (see Section 2.6.1.14) or flow observations (Section 2.6.7.3) have been defined. Select this menu item to open a Scatter Diagram dialog box, which is identical as the Scatter Diagram (Hydraulic Head) dialog box as described in Section 2.6.1.20 with two exceptions:

- The user-specified observation times and observed values are given in the columns *Simulation Time* and *Observed Value* directly without interpolating to the times at the end of each stress period or time step. The Calculated Value column contains the values calculated by MODFLOW-2000, i.e., the values are not calculated by pmp using equation 2.34.
- A *Result Type* option appears in the Data tab. The first result type is "Observed values versus simulated values". When the second result type "Weighted observed values versus weighted simulated values" is chosen, the observed and calculated values are multiplied by a weighting factor, which is the square root of weight defined in the Option tab of the Head Observations (Fig. 4.36) or Flow Observation (Fig. 2.75) dialog boxes.

MODFLOW-2000 (Parameter Estimation) | View | Time-Series Curves

This menu item is available only if head observations (see Section 2.6.1.14) or flow observations (Section 2.6.7.3) have been defined. Select this menu item to open a Time-Series Curves dialog box, which is identical as the Time-Series Curves (Hydraulic Head) dialog box as described in Section 2.6.1.20. The only exception is that the user-specified observation times and observed values are given in the columns *Simulation Time* and *Observed value* directly without interpolating to the times at the end of each stress period or time step. The *Calculated Value* column contains the values calculated by MODFLOW-2000, i.e., the values are not calculated by **PM** using equation 2.34 (page 79).

2.6.8 PEST (Parameter Estimation)

This menu provides an interface between **PM**, MODFLOW and PEST. All versions of MODFLOW, can be used with PEST. The parameters and/or excitations, which may be estimated by regression, are listed in Table 2.9. The adjustable aquifer parameters depend on the selection of BCF or LPF package, and layer types.
During a parameter estimation process, PEST searches optimum parameter values for which the sum of squared deviations between model-calculated and observed values of hydraulic heads or drawdowns at the observation boreholes is reduced to a minimum. The coordinates of the observation boreholes and observed values are given in *PEST (Parameter Estimation)* | *Head Observations* (or *Drawdown Observations*). Note that a simultaneous fit of highly correlated parameters, for example transmissivity and recharge values on the basis of observed heads or drawdowns only, is of little value in steady-state problems due to the non-uniqueness of such a fit. The parameters to be estimated are defined in the following steps.

► To define an adjustable parameter for estimation

1. Select a parameter from the *Parameters* menu or select a package from the *Models (Flow Simulation)* | *MODFLOW* | *Flow Packages* menu, for example Transmissivity or Well.

2. Assign an initial guess of the parameter value and a parameter number to cells within an area where the parameter value should be estimated. The parameter number needs to be unique within a parameter type (e.g., T, S or Ss) and may be any integer ranging between 1 and 500. Set the parameter number to zero, if the specified parameter value should not be estimated.
3. Select *PEST (Parameter Estimation)* | *Simulation Settings* to open a Simulation Settings (PEST) dialog box, which provides an overview of all parameters defined in previous steps and interfaces for setting control parameters. The dialog box also allows selecting or deselecting parameters for estimation (see Section 2.6.8.1).

Note.

1. Using the Calculated settings in the Layer Options dialog box, **PM** allows the user to specify HK, VK or Ss instead of T, VCONT and S values to layers of types 0 or 2. However, when using PEST to estimate T, VCONT or S values, the user must define the adjustable parameters by selecting Transmissivity, Vertical Leakance or Storage Coefficient from the Parameters menu, regardless whether the Calculated or User-Specified settings are used.
2. To estimate the conductance values of head-dependent cells (e.g., drain, general head-boundary, river or stream cells) or pumping rates of wells, a non-zero conductance value or pumping rate must be assigned to those cells with adjustable parameters. Conductance values or pumping rates will not be adjusted, if the user-specified cell values are zero.

Table 2.9 Adjustable parameters through PEST within **PM**

Packages	**Abbreviation**	**Adjustable Parameters**
Block-Centered Flow	BCF	Layer type 0: T, S, and VCONT Layer type 1: HK, Sy, and VCONT Layer type 2: T, S, Sy, and VCONT Layer type 3: HK, S, Sy and VCONT
Layer-Property Flow	LPF	All layer types: HK, HANI, VANI, VK, Ss, and Sy
Drain	DRN	Conductance of drain cells
Evapotranspiration	EVT	Maximum evapotranspiration rate
General-Head Boundary	GHB	Conductance of GHB cells
Horizontal Flow Barrier	HFB6	Hydraulic characteristic of barrier
Interbed Storage	IBS	Inelastic storage factor
Recharge	RCH	Recharge flux
Reservoir	RES	Conductance of RES cells
River	RIV	Conductance of RIV cells
Stream-Flow Routine	STR	Conductance of STR cells
Well	WEL	Pumping or injection rates of WEL cells

2.6.8.1 PEST (Parameter Estimation) | Simulation Settings

The required inputs and options for running PEST are specified in the Simulation Settings (PEST) dialog box (Fig. 2.79). The names of most input variables of this dialog box are inherited from the PEST manual[37] and the Addendum to the PEST Manual[39], which provide a great inside into to the theory and application of PEST. The user is encourage to download and consult these references as needed. The Operation Mode dropdown box Fig. 2.79is used to define how PEST should run and the rest of the available settings are grouped under six tabs described in the following sections below. The functions of Operation Mode dropdown box and the push buttons are defined as follows.

- *Operation Mode*:
  - Parameter Estimation: PEST will use the available information to estimate parameters defined in the Parameters Tab by running the model as many times as needed.
  - Sensitivity Analysis: When this option is selected, the maximum number of optimization iterations (see NOPTMAX in the Control Data tab) will be set to -1. PEST will run in the Parameter Estimation mode, but will terminate execution immediately after it has calculated the Jacobian matrix for the first time. The parameter covariance, correlation coefficient and eigenvector matrices will be written to the run record file, and parameter sensitivities will be written to the sensitivity file; these are based on the initial parameter set defined in the Parameters tab.
  - Forward Model Run using PARVAL values given in the Parameters tab: When this option is selected, the maximum number of optimization iterations (see NOPTMAX in the Control Data tab) will be set to 0. PEST will run in the Parameter Estimation mode, but will not calculate the Jacobian matrix. Instead it will terminate execution after just one model run. This setting can thus be used when you wish to calculate the objective function corresponding to a particular parameter set and/or to inspect observation residuals corresponding to that parameter set.
  - Regularization: Within each optimization iteration PEST's task when working in regularization mode is identical to its task when working in parameter estimation mode, i.e., it must minimize an objective function using a linearized version of the model encapsulated in a Jacobian matrix. However just before calculating the parameter upgrade vector, PEST calculates the appropriate "regularization weight factor" to use for that iteration. This is the factor by which all of the weights pertaining to regularization information are multiplied (in accordance with equation 2.33 of the PEST manual [37]) prior to formulating the overall objective function whose task it is for PEST to minimize on that iteration. As parameters shift and the Jacobian matrix changes (an outcome of the nonlinear nature of most models), the regularization weight factor also changes. Hence it needs to be re-calculated during every optimization iteration.

Use of PEST in regularization mode is fully described in Chapters 7 and 8 of the PEST manual. The user is required to supply control variables listed in the Regularization tab and to supply at least one prior information equation with the name of observation group ($Obgnme$) set to "regul".

- *Save* and *Load*: Using the Save button, the user can save the settings in separate files, which can be loaded at a later time by using the Load button.
- *Update*: Click the Update button to retrieve the estimated parameter values, saved in the PESTCTL.PAR file that contains the estimated parameter values. PESTCTL.PAR is created by PEST after running it in the parameter estimation mode. The Update button is disabled and dimmed, if this file is not available.

The Parameters Tab

The Parameters Tab contains a table that gives an overview of the initial values and properties of estimated parameters. The initial value (PARVAL) of parameter is the arithmetical mean of the cell values of that parameter. The parameter's lower bound PARLBND and upper bound PARUBND default to two orders lower andhigher than PARVAL, respectively.

If a parameter is removed by changing the parameter number to zero in the Data Editor, the corresponding parameter in the table is ignored. **PM** does not delete that adjustable parameter from the table. To delete the parameter, click on its record selector (▭ before the first column of the table), then press the *Del* key. Note that the user cannot manually add a parameter to the table. If a parameter is deleted by mistake, simply click the Cancel button to discard all changes, or click the OK button to

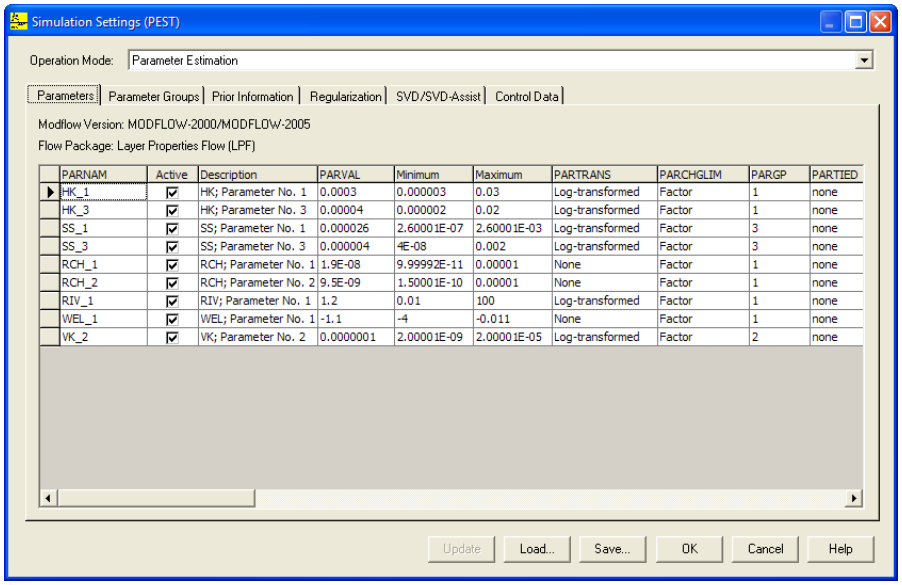

Simulation Settings (PEST)
Operation Mode: Parameter Estimation
Parameters
Parameter Groups
Prior Information
Regularization
SVD/SVD-Assist
Control Data
Modflow Version: MODFLOW-2000/MODFLOW-2005
Flow Package: Layer Properties Flow (LPF)
PARNAM Active Description PARVAL Minimum Maximum PARTRANS PARCHGLIM PARGP PARTIED
HK_1 HK; Parameter No. 1 0.0003 0.000003 0.03 Log-transformed Factor 1 none
HK_3 HK; Parameter No. 3 0.00004 0.000002 0.02 Log-transformed Factor 1 none
SS_1 SS; Parameter No. 1 0.000026 2.60001E-07 2.60001E-03 Log-transformed Factor 3 none
SS_3 SS; Parameter No. 3 0.000004 4E-08 0.002 Log-transformed Factor 3 none
RCH_1 RCH; Parameter No. 1 1.9E-08 9.99992E-11 0.00001 None Factor 1 none
RCH_2 RCH; Parameter No. 2 9.5E-09 1.50001E-10 0.00001 None Factor 1 none
RIV_1 RIV; Parameter No. 1 1.2 0.01 100 Log-transformed Factor 1 none
WEL_1 WEL; Parameter No. 1 -1.1 -4 -0.011 None Factor 1 none
VK_2 VK; Parameter No. 2 0.0000001 2.00001E-09 2.00001E-05 Log-transformed Factor 2 none
Update
Load...
Save...
OK
Cancel
Help

Fig. 2.79. The Simulation Settings (PEST) dialog box

accept changes, and then open the Simulation Settings (PEST) dialog box again to recover the ”lost” parameter.

The meaning of each column of the table is described below. By clicking on a column header, the parameters can be sorted in ascending order using the values of that column.

- *PARNAM*: While editing data of a certain aquifer parameter or flow package, the spatial extent of an adjustable parameter is defined by assigning a parameter number to the cells of interest. PARNAM is a combination of that parameter number and the short name of the aquifer parameter (i.e., HK, HANI, VK, VANI, SS, SY, T, S or VCONT) or package. For example, if parameter numbers 1 and 2 are specified for the Recharge package, then RCH_1 and RCH_2 are assigned to PARNAM (Fig. 2.79). Modification of the assigned names is not allowed.
- *Active*: The value of an estimated parameter will only be adjusted if Active is checked. Otherwise the user-specified cell value will be used for the simulation. When switching from the BCF to LPF (or from LPF to BCF) package, some aquifer parameters might become unadjustable (e.g., T, S are not adjustable when using the LPF package), and they will be indicated by gray background color. Normally, the total number of active parameters should not exceed 10, although **PM** allows 500 parameters.
- *Description*: A text describing the parameter can be entered here (optional), for example, ”recharge zone one”. A maximum of 120 characters is allowed.
- *PARVAL1* is a parameter's initial value. For a fixed parameter, this value remains invariant during the optimization process. For a tied parameter (see PARTRANS below), the ratio of PARVAL1 to the parent parameter's PARVAL1 sets the ratio between these two parameters to be maintained throughout the optimization process. For an adjustable parameter, PARVAL1 is the parameter's starting value which, together with the starting values of all other adjustable parameters, it is successively improved during the optimization process. To enhance optimization efficiency, the user should choose an initial parameter value, which is close to the guessed optimized value. The user should note the following repercussions of choosing an initial parameter value of zero.
  - Limitation of the parameter adjustment is not possible (see the discussion on RELPARMAX and FACPARMAX) during the first optimization iteration if the starting value of a parameter is zero. Furthermore FACORIG cannot be used to modify the action of RELPARMAX and FACPARMAX for a particular parameter throughout the optimization process, if that parameter's original value is zero.
  - A relative increment for derivatives calculation cannot be evaluated during the first iteration for a parameter whose initial value is zero. If the parameter belongs to a group for which derivatives are, in fact, calculated as Relative (see INCTYP and DERINC below), a non zero DERINCLB variable must be provided for that group.

  - If a parameter has an initial value of zero, the parameter can be neither a tied nor a parent parameter, as the tied/parent parameter ratio cannot be calculated.
- *PARLBND* and *PARUBND* are a parameter's lower and upper bounds respectively. For adjustable parameters the initial parameter value (PARVAL1) must lie between these two bounds. For fixed and tied parameters, PARLBND and PARUBND are ignored.
- *PARTRANS* controls the parameter transformation. By clicking on a cell of the PARTRANS column, this flag can be set as None, Log-transformed, Tied or Fixed. Use Log-transformed, if you wish that a parameter be log transformed throughout the estimation process, this is recommended for transmissivities and hydraulic conductivities. A parameter, which can become zero or negative in the course of the parameter estimation process, must not be log transformed; hence if a parameter's lower bound is zero or less, PEST will disallow logarithmic transformation for that parameter. Note that by using an appropriate scale and offset, you can ensure that parameters never become negative. Thus if you are estimating the value for a parameter whose domain, as far as the model is concerned, is the interval [-9.99, 10], you can shift this domain to [0.01, 20] for PEST by designating a scale of 1.0 and an offset of -10.0. Similarly if a parameter's model domain is entirely negative, you can make this domain entirely positive for PEST by supplying a scale of -1.0 and an offset of 0.0. See the discussion on the SCALE and OFFSET variables below.
  If a parameter is fixed, taking no part in the optimization process, PARTRANS must be specified as Fixed. If a parameter is linked to another parameter, this is signified by a PARTRANS value of Tied. In the latter case the parameter plays only a limited role in the estimation process. However the parameter to which the tied parameter is linked (this "parent" parameter must be neither fixed nor tied itself) takes an active part in the parameter estimation process; the tied parameter simply "piggy backs" on the parent parameter, the value of the tied parameter maintaining at all times the same ratio to the parent parameter as the ratio of their initial values. If a parameter is neither fixed nor tied, and is not log transformed, the parameter transformation variable PARTRANS must be supplied as None.
- *PARCHGLIM* is used to designate whether an adjustable parameter is relative-limited or factor-limited (See the discussion on RELPARMAX and FACPARMAX; page 169). For tied or fixed parameters PARCHGLIM has no significance.
- *PARGP* is the number of the group to which a parameter belongs. Parameter groups are discussed in Group Definitions below.
- *PARTIED* is the name of the "parent" parameter to which the parameter is tied. You can select a name from a drop down list.
- *SCALE* and *OFFSET*: Just before a parameter value is written to an input file of MODFLOW, it is multiplied by the real variable SCALE, after which the real variable OFFSET is added. The use of these two variables allows you to redefine the domain of a parameter. Because they operate on the parameter value "at the last moment" before it is sent, they take no part in the estimation process; in fact

they can ”conceal” from PEST the true value of a parameter as seen by the model, PEST optimizing, instead, the parameter bp where

$$b_p = (b_m - offset)/scale \tag{2.59}$$

Here b_p is the parameter optimized by PEST, b_m is the parameter seen by the model, while $scale$ and $offset$ are the scale and offset values for that parameter respectively. If you wish to leave a parameter unaffected by scale and offset, enter the SCALE as 1.0 and the OFFSET as 0.0.

The Parameter Groups Tab

In PEST, the input variables that define how derivatives are calculated pertain to parameter groups rather than to individual parameters. These input variables are specified in the Parameter Groups tab of the Simulation Settings (PEST) dialog box (Fig. 2.80). Thus derivative data do not need to be entered individually for each parameter; however, if you wish, you can define a group for every parameter and set the derivative variables for each parameter separately. In many cases parameters fall neatly into separate groups which can be treated similarly in terms of calculating derivatives.

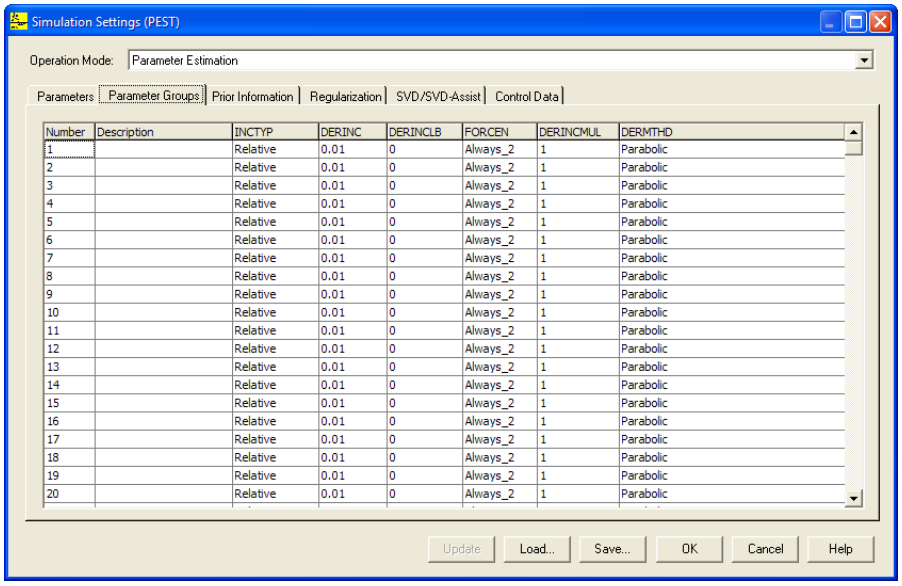

Simulation Settings (PEST)
Operation Mode: Parameter Estimation
Parameters
Parameter Groups
Prior Information
Regularization
SVD/SVD-Assist
Control Data
Number Description INCTYP DERINC DERINCLB FORCEN DERINCMUL DERMTHD
1 Relative 0.01 0 Always_2 1 Parabolic
2 Relative 0.01 0 Always_2 1 Parabolic
3 Relative 0.01 0 Always_2 1 Parabolic
4 Relative 0.01 0 Always_2 1 Parabolic
5 Relative 0.01 0 Always_2 1 Parabolic
6 Relative 0.01 0 Always_2 1 Parabolic
7 Relative 0.01 0 Always_2 1 Parabolic
8 Relative 0.01 0 Always_2 1 Parabolic
9 Relative 0.01 0 Always_2 1 Parabolic
10 Relative 0.01 0 Always_2 1 Parabolic
11 Relative 0.01 0 Always_2 1 Parabolic
12 Relative 0.01 0 Always_2 1 Parabolic
13 Relative 0.01 0 Always_2 1 Parabolic
14 Relative 0.01 0 Always_2 1 Parabolic
15 Relative 0.01 0 Always_2 1 Parabolic
16 Relative 0.01 0 Always_2 1 Parabolic
17 Relative 0.01 0 Always_2 1 Parabolic
18 Relative 0.01 0 Always_2 1 Parabolic
19 Relative 0.01 0 Always_2 1 Parabolic
20 Relative 0.01 0 Always_2 1 Parabolic
Update
Load...
Save...
OK
Cancel
Help

Fig. 2.80. The Parameter Groups tab of the Simulation Settings (PEST) dialog box

- *Number* is the group number. The maximum number of parameter groups is 150.
- *Description*: A text describing the estimated parameter can be entered here (optional), for example, ”Transmissivity Group 1”. A maximum of 120 characters is allowed.

- *INCTYP* and *DERINC*: INCTYP defines the type of parameter increment (perturbation) used for forward difference calculation of derivatives with respect to any parameter belonging to the group. INCTYP can be Relative, Absolute or Rel_to_max.
  - *INCTYP* = *Relative*: The parameter increment is calculated as a fraction of the current value of that parameter; that fraction is specified in DERINC. A DERINC value of 0.01 is often appropriate.
  - *INCTYP* = *Absolute*: The parameter increment is fixed at the value of DERINC. No suggestion for an appropriate DERINC value can be provided for this option; the most appropriate increment will depend on the parameter magnitudes.
  - *INCTYP* = *Rel_to_max*: The parameter increment is calculated as a fraction of the group member with highest absolute value, that fraction again being DERINC. A DERINC value of 0.01 is often appropriate. If a group contains members, which are fixed and/or tied, the user should note that the values of these parameters are taken into account when calculating parameter increments.
- *DERINCLB* is the absolute lower limit of parameter increments for all group members. If a parameter increment is calculated as Relative, it may become too low if the parameter values become very small. And, if a parameter increment is calculated as Rel_to_max, it may become too low if the modulus of the largest parameter in the group is very small. A parameter increment be-comes "too low" if it does not allow reliable derivatives to be calculated with respect to that parameter because of round off errors incurred in the subtraction of nearly equal model generated values. DERINCLB is used to bypass this possibility.
  Set DERINCLB to zero if the user does not wish to place a lower limit on parameter increments in this fashion. Note that if INCTYP is Absolute, DERINCLB is ignored.
- *FORCEN* can be Always_2, Always_3 or Switch. It determines how to calculate derivatives for group members.
  - *FORCEN* = *Always_2*: Derivatives for all parameters belonging to that group will always be calculated using the forward difference method.
  - *FORCEN* = *Always_3*: PEST will use the central difference method to calculate the derivatives. In this case, twice as many model runs as there are parameters within the group will be required; however the derivatives will be calculated with greater accuracy and this will probably have a beneficial effect on the performance of PEST.
  - *FORCEN* = *Switch*: Derivatives calculations for all adjustable group members will begin using the forward difference method, switching to the central method for the remainder of the estimation process after the relative objective function reduction between successive iterations is less than PHIREDSWH as defined in the Control Data below.

  Experience has shown that in most instances the most appropriate value for FORCEN is Switch. This allows speed to take precedence over accuracy in the early stages of the optimization process when accuracy is not critical to objective

function improvement, and accuracy to take precedence over speed later in the process when realization of a (normally smaller) objective function improvement requires that derivatives be calculated with as much accuracy as possible, especially if parameters are highly correlated and the normal matrix thus approaches singularity.

- *DERINCMUL*: If a three point derivatives calculation is employed, the value of DERINC is multiplied by DERINCMUL. Set DERINCMUL to a value of 1.0 if the user does not wish the parameter increment DERINC to be changed. Alternatively, if for some reason the user wishes the increment to be reduced if three point derivatives calculation is employed, DERINCMUL should be less than 1.0. Experience shows that a value between 1.0 and 2.0 is usually satisfactory.
- *DERMTHD* defines the variant of the central (i.e. three point) method used for derivatives calculation and is used only when FORCEN is Always_3 or Switch. PEST provides three variants: Parabolic, Best_fit or Outside_pts. Refer to the manual of PEST for details about these methods.

The Prior Information Tab

It often happens that we have some information concerning the parameters that we wish to optimize, and that we obtained this information independently of the current experiment. This information may be in the form of other unrelated estimates of some or all of the parameters, or of relationships between parameters. It is often useful to include this information in the parameter estimation process because it may lend stability to the process.

To define prior information, first check the *Active* box in the Prior Information tab, and then enter the prior information equation in the Prior Information column. The syntax of a prior information equation is

$$Pilbl \;\; Pifac * Parnme + Pifac * \log(Parnme) \ldots = Pival \; Weight \; Obgnme \tag{2.60}$$

The variables of the prior information equations are defined as follows. All variables and symbols must be separated from by at least one space.

- $Pilbl$: Each prior information article must begin with a case insensitive prior information label. The label must be no more than twenty characters in length and must be unique to each prior information article.
- $Pifac$ and $Parnme$: $Pifac$ is a parameter factor. $Parnme$ is parameter name. Both are required. To the left of the "=" sign there are one or more combinations $Pifac$ and $Parnme$, with a "log" prefix to $Parnme$ if appropriate. $Pifac$ and $Parnme$ are separated by a "*" character signifying multiplication. All parameters referenced in a prior information equation must be adjustable parameters; i.e., you must not include any fixed or tied parameters in an article of prior information. Furthermore, any particular parameter can be referenced only once in any one prior information equation; however, it can be referenced in more than one equation.

- $Pival$: $Pival$ is the value of the right side of the prior information equation.
- $Weight$: $Weight$ is the weight assigned to the article of prior information in the parameter estimation process. The prior information weight should ideally be inversely proportional to the standard deviation of $Pival$; it can be zero if you wish but must not be negative. In practice the weights should be chosen such that the prior information equation neither dominates the objective function or is dwarfed by other components of the objective function. In choosing observation and prior information weights, remember that the weight is multiplied by its respective residual and then squared before being assimilated into the objective function.
- $Obgnme$: $Obgnme$ is observation group to which the prior information belongs and $Obgnme$ must be twelve characters or less in length. **When running PEST in the Regularization mode (see Regularization tab below)** $Obgnme$ **of at least one of the prior information equations must be "regul". PEST can accommodate multiple regularization groups. Any observation group name** $Obgnme$ **begins with the letters "regul" is considered to be a regularization group. See Sec. 8.2 of the PEST manual for details about multiple regularization groups.**

Some examples of prior information equations are given below, refer to the PEST manual [37] for more details.

The parameter factor must never be omitted. Suppose, for example, that a prior information equation consists of only a single term, viz. that an untransformed, adjustable parameter named "par1" has a preferred value of 2.305, and that you would like PEST to include this information in the optimization process with a weight of 1.0. If this article of prior information is given the label "pi1", the pertinent prior information line can be written as

```
pi1 1.0 * par1 = 2.305 1.0 pr_info
```

If a parameter is log-transformed, you must provide prior information pertinent to the log of that parameter, rather than to the parameter itself. Furthermore, the parameter name must be placed in brackets and preceded by "log" (note that there is no space between "log" and the following opening bracket). Thus, in the above example, if parameter "par1" is log-transformed, the prior information article should be rewritten as

```
pi1 1.0 * log(par1) = .362671 1.0 pr_info
```

Note that logs are taken to base 10. Though not illustrated, you will also need to review the weight which you attach to this prior information article by comparing the extent to which you would permit the log of "par1" to deviate from 0.362671 with the extent to which model-generated observations are permitted to deviate from their corresponding measurements. The left side of a prior information equation can be comprised of the sum and/or difference of a number of factor-parameter pairs of the type already illustrated; these pairs must be separated from each other by a "+" or "-" sign, with a space to either side of the sign. For example:

```
pi2 1.0 * par2 + 3.43435 * par4 - 2.389834 * par3 =
                                1.09e3 3.00 group_pr
```

Prior information equations which include log-transformed parameters must express a relationship between the logs of those parameters. For example if you would like the ratio between the estimated values of parameters "par1" and "par2" to be about 40.0, the prior information article may be written as

```
pi3 1.0 * log(par1) - 1.0 * log(par2) = 1.60206 2.0 group_pr
```

The Regularization Tab

Tikhonov regularization is the most commonly used method of regularization and is incorporated in PEST. In its broadest sense, *regularization* is a term used to describe the process whereby a large number of parameters can be simultaneously estimated without incurring the numerical instability that normally accompanies parameter non-uniqueness. Numerical stability is normally achieved through the provision of *supplementary information* to the parameter estimation process. Such *supplementary information* often takes the form of preferred values for parameters, or for relationships between parameters (i.e., prior information). Thus if, for a particular parameter, the information content of the observation dataset is such that a unique value cannot be estimated for that parameter on the basis of that dataset alone, uniqueness can nevertheless be achieved by using the supplementary information provided for that parameter through the regularization process.

Regularization is particularly useful in estimating values for parameters which describe the spatial distribution of some property over a two- or three-dimensional model domain of a ground water model. The user is no longer required to subdivide the model domain into a small number of zones of piecewise parameter constancy. Rather, a large number of parameters can be used to describe the distribution of the spatial property and PEST's regularization functionality can be used to estimate values for these parameters.
To run PEST in the regularization mode, select Regularization from the *Operation Mode* drop-down box, assign appropriate control parameters to the Regularization tab of of the Simulation Settings (PEST) dialog box (Fig. 2.81). **You must also define at least one prior information equation (see above) and set the observation group (**$Obgnme$**) of the prior information equation to "regul"**. Refer to chapter 7 of the PEST manual [37] for further details about regularization.

- *Target measurement objective function (PHIMLIM)*:
  This is the upper limit of the measurement objective function (i.e., the upper level of model-to-measurement misfit) that is tolerable when trying to minimize the regularization objective function. In some cases a PEST regularization run will postdate a normal parameter estimation run. If the latter run was successful, it will have informed the user of how low the measurement objective function can be if all parameters are adjusted without reference to any regularization conditions. PHIMLIM should be set somewhat above this, for the imposition of reg-

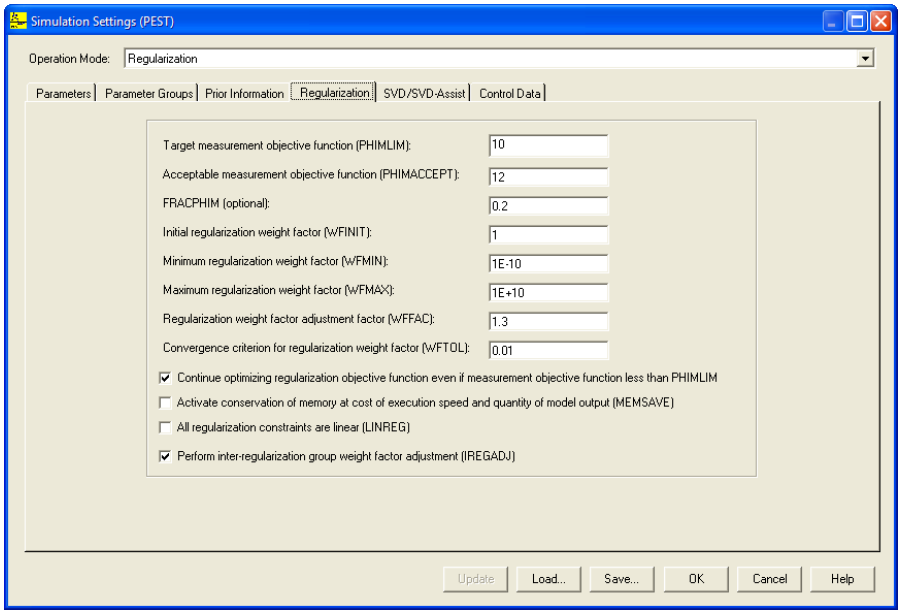

Simulation Settings (PEST)
Operation Mode: Regularization
Parameters
Parameter Groups
Prior Information
Regularization
SVD/SVD-Assist
Control Data
Target measurement objective function (PHIMLIM): 10
Acceptable measurement objective function (PHIMACCEPT): 12
FRACPHIM (optional): 0.2
Initial regularization weight factor (WFINIT): 1
Minimum regularization weight factor (WFMIN): 1E-10
Maximum regularization weight factor (WFMAX): 1E+10
Regularization weight factor adjustment factor (WFFAC): 1.3
Convergence criterion for regularization weight factor (WFTOL): 0.01
Continue optimizing regularization objective function even if measurement objective function less than PHIMLIM
Activate conservation of memory at cost of execution speed and quantity of model output (MEMSAVE)
All regularization constraints are linear (LINREG)
Perform inter-regularization group weight factor adjustment (IREGADJ)
Update
Load...
Save...
OK
Cancel
Help

Fig. 2.81. The Regularization tab of the Simulation Settings (PEST) dialog box

ularization constraints will mostly result in a slight diminution of PEST's ability to fit the field data exactly.

- *Acceptable measurement objective function (PHIMACCEPT)*:
  During each optimization iteration, just after it has linearized the problem through calculating the Jacobian matrix, and just before it begins calculation of the parameter upgrade vector, PEST calculates the optimal value of the regularization weight factor for that iteration. This is the value which, under the linearity assumption encapsulated in the Jacobian matrix, results in a parameter upgrade vector for which the measurement component of the objective function is equal to PHIMLIM. However, due to the approximate nature of the linearity assumption, PEST may not be able to lower the measurement component of the objective function to PHIMLIM on that iteration in spite of the fact that it uses a number of different values for the Marquardt lambda in attempting to do so. If it cannot lower the measurement objective function to an acceptable level, it simply accepts the upgraded parameters, proceeds to the next optimization iteration and tries again. However if it does succeed in lowering the measurement objective function to an acceptable level, or if it has succeeded in doing this on previous iterations, then PEST slightly alters its philosophy of choosing new Marquardt lambdas, in that it now attempts to lower the regularization component of the objective function while maintaining the measurement component of the objective function below this acceptable level. This acceptable level is PHIMACCEPT; it should be set slightly higher than PHIMLIM in order to give PEST some "room to move".

- *FRACPHIM (Optional)*:
  PEST ignores the value supplied for FRACPHIM unless it is greater than zero. A value of between zero and 1.0 (but normally less than about 0.3) can be supplied for this variable if you are unsure what value to use for PHIMLIM. See Section 7.3.4 of the PEST manual [37] for a full discussion of this variable.
- *Initial regularization weight factor (WFINIT)*: This is the initial regularization weight factor. During every optimization iteration PEST calculates a suitable regularization weight factor to use during that optimization iteration using an iterative, numerical solution procedure; its initial value when implementing this procedure for the first optimization iteration is WFINIT.
- *Minimum regularization weight factor (WFMIN) and Maximum regularization weight factor (WFMAX)*: These are the minimum and maximum permissible values that the regularization weight factor is allowed to take. If a regularization scheme is poor, (and does not lend too much stability to an already unstable parameter estimation process), selection of appropriate values for WFMIN and WFMAX may be quite important, for these can prevent PEST from calculating outrageous values for the regularization weight factor in an attempt to compensate for inadequacies of the regularization scheme.
- *Regularization weight factor adjustment factor (WFFAC) and Convergence criterion for regularization weight factor (WFTOL)*:
  When PEST calculates the appropriate regularization weight factor to use during any optimization iteration, it uses an iterative procedure which begins at the value of the regularization weight factor calculated for the previous optimization iteration; for the first optimization iteration it uses WFINIT to start the procedure. In the process of finding the weight factor which will result in a measurement objective function of PHIMLIM, PEST first travels along a path of progressively increasing or decreasing weight factor. In undertaking this exploration, it either multiplies or divides the weight factor by WFFAC; it continues to do this until it has found two successive weight factors which lie on either side of the optimal weight factor for that optimization iteration. Once it has done this, it uses Newtons method to calculate the optimal weight factor, through a series of successive approximations. When two subsequent weight factors calculated in this way differ from each other by no more than a relative amount of WFTOL, the optimal weight factor is deemed to have been calculated.
- *Continue optimizing regularization objective function even if measurement objective function less than PHIMLIM*:
  Under normal circumstances, when working in regularization mode, PEST ceases execution immediately if the measurement objective function falls below PHIMLIM. There are some circumstances, however, where minimization of the regularization objective function is just as important as allowing the measurement objective function to reach PHIMLIM. If this box is checked the variable REGCONTINUE of the PEST control data file will be as ”continue” to ensure that PEST will continue optimizing regularization objective function after reached PHIMLIM.

- *Activate conservation of memory at cost of execution speed and quantity of model output (MEMSAVE)*: If this box is checked the variable MEMSAVE of the PEST control data file will be set as "memsave" and Nonessential PEST tasks which are curtailed include the following:
  - The parameter covariance matrix, and matrices derived from it, are not calculated by PEST at regular intervals during the parameter estimation process for recording in the matrix file, case.mtt; nor are these matrices calculated at the end of the inversion process for recording in the run record file case.rec. Because the covariance matrix is unavailable, parameter uncertainties cannot be calculated, and hence are also not recorded in the run record file. (In a regularization context these have little meaning anyway.)
  - Some avenues for increasing the efficiency of regularization calculations are no longer available under the leaner storage regime that prevails when memory conservation is active (including the benefits gained through the LINREG variable and through the placing of regularization observations behind other observations involved in the parameter estimation process). This can lead to significant run-time penalties in problems involving many parameters; unfortunately, these are the very contexts in which memory conservation is most likely to be warranted.
- *All regularization constraints are linear (LINREG)*: If this box is checked the variable LINREG of the PEST control data file will be set to "linreg". As is discussed in chapter 7 of the PEST manual [37], regularization constraints can be supplied through observations, through prior information, or through both of these mechanisms. Prior information relationships are always linear. Regularization constraints supplied as observations (for which the current value of pertinent relationships is calculated by the model), can be linear or nonlinear; in either case, derivatives of these relationships with respect to adjustable parameters are re-evaluated by PEST during each optimization iteration. If regularization information is entirely linear, there are many matrix operations carried out as part of PEST's regularization functionality which do not need to be repeated from iteration to iteration. If repetition of these calculations can be avoided in parameter estimation contexts involving many regularization constraints, significant gains in efficiency can be made.
- *Perform inter-regularization group weight factor adjustment (IREGADJ)*: If this box is checked the variable MEMSAVE of the PEST control data file will be set to 1. In this case, PEST takes account of both the number and sensitivities of regularization observations and prior information equations in each group in determining relative inter-regularization group weighting, so that the contribution made by each group to the overall set of regularization constraints is balanced.

The SVD/SVD-Assist Tab

SVD - Truncated Singular Value Decomposition

Truncated singular value decomposition (i.e., truncated SVD) is another popular method of solving inverse problems. Using SVD, the dimensionality of parameter space is reduced to that point at which a unique solution to the parameter estimation problem is possible. Furthermore this simplification is carried out in a way that is mathematically optimal with respect to the dataset available for calibration. Thus it effectively allows the estimation of parameter combinations rather than parameters themselves, these combinations being such as to be most receptive to the data at hand. In this way, the problem simplification necessary to achieve numerical stability of the parameter estimation process, is undertaken by the process itself. Furthermore, the inclusion of many parameters in the model calibration process can be justified by observing that the inclusion of such parameterization detail allows the truncated SVD mechanism more flexibility in determining an appropriate simplification strategy than by undertaken preemptive simplification through reducing the number of model parameters externally to the parameter estimation process.

The required settings for using PEST's SVD functionality are given in the *SVD - Truncated Singular Value Decomposition* group of Fig. 2.82 and are explained below.

- *Activate SVD for solution of inverse problem*: Check this box to activate PEST's SVD functionality.
- *Set PEST variables RLAMBDA1 to zero and NUMLAM to one*: Check this box to set Marquardt lambda (RLABMDA1) and the number of trial lambdas (NUMLAM) to the values recommended by the PEST manual.
- *Create complete SVD output file (uncheck this box to save only eigenvalues to the output file)* When SVD is activated, PEST writes a file named *modelname.svd* in

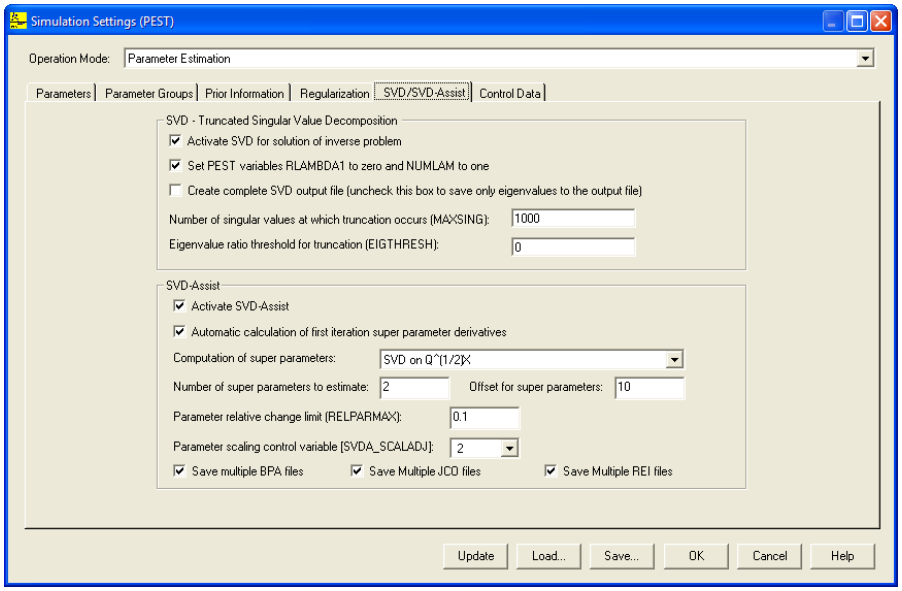


Fig. 2.82. The SVD/SVD-Assist tab of the Simulation Settings (PEST) dialog box

addition to its normal output files. This contains singular values (arranged in decreasing order) and corresponding eigenvectors computed on each occasion that singular value decomposition is carried out. It also records the number of singular values that are actually used in computation of the parameter upgrade vector (i.e., the number of singular values remaining after truncation). Singular value decomposition is carried out at least once per iteration (corresponding to the testing of different Marquardt lambdas - including the sole Marquardt lambda value of zero if RLAMBDA1 is set to zero and NUMLAM is set to 1 as suggested above); multiple incidences of singular value decomposition are required in any optimization iteration in which parameters hit their bounds.
The SVD output file can become very large; not all of the information contained in it is always worth reading. However an inspection of singular values can often provide assistance in determining best values for MAXSING and EIGTHRESH (see below). By clearing this box, only singular values (and not their corresponding eigenvectors), are written to *modelname.svd*, thus reducing its size considerably. The number of singular values used during each parameter upgrade is also recorded.

- *Number of singular values at which truncation occurs (MAXSING)*: In other words, MAXSING is the maximum number of singular values to include in the inversion process (equivalent to the maximum number of eigenvalues, and the maximum number of degrees of freedom in parameter solution space). This is problem-dependent. Experience with a particular problem may dictate its optimal value; set it high enough to obtain a good fit between model outputs and field data, but not so high that numerical instability or "overfitting" of model outputs to measurements occurs, resulting in unrealistic parameter values. Alternatively, set MAXSING very high (for example, equal to the number of estimable parameters) and let EIGTHRESH determine the number of singular values employed in the parameter estimation process.
- *Eigenvalue ratio threshold for truncation (EIGTHRESH)*: EIGTHRESH is the ratio of lowest to highest eigenvalue at which truncation is implemented; this then determines the number of singular values that are used in the inversion process, for only those singular values are used whose ratio to the maximum singular value is above this threshold. Limited experience to date indicates that 10^{-6} or 10^{-7} is a good setting for EIGTHRESH; set it higher (e.g., 10^{-5}) if numerical instability or over-fitting occurs.

SVD-Assist

SVD-Assist is a hybrid method which combines the strengths of the Tikhonov and SVD regularization methods, while accomplishing enormous gains in efficiency, is described in this section. Although truncated SVD can be used with Tikhonov regularization, this process is not expected to be as efficient as the SVD-assist methodology. It is fairly easy to setup a SVD-Assisted run with the help of **PM**. The user is encouraged to consult Sec. 8.5 of the PEST manual [37] for detailed explanation of

the mechanism of SVD-assisted parameter estimation. The available settings of the *SVD-Assist* group of Fig. 2.82 are listed below.

- *Activate SVD-Assist*:
  Check this box to enable SVD-assisted parameter estimation. With SVD-Assist activated, **PM** will create two PEST control files, namely *pre-svda.pst* and *base-svda.pst*, prior to running PEST. The former is used for the purpose of derivatives calculation by a pre-SVD-assist PEST run. The latter is used by the utility program SVDAPREP (which is a part of PEST) to create a third PEST control file used for the estimation of super parameters. **PM** will also create a batch file called *pest.bat* which encapsulates the individual steps of an SVD-assisted PEST run as follows:
  1. *Commence a pre-SVD-assist PEST Run*:
     Copy *presvda.pst* to *svda.pst* and then run PEST with *svda.pst*. This step will create a file called *svda.jco* storing the Jacobian matrix.
  2. *Execute SVDAPREP*:
     Copy *basesvda.pst* to *svda.pst* and then run SVDAPREP.EXE to generate the third PEST control file *pestctl.pst* based on *svda.pst* and a new batch file *svdabatch.bat*. The required input data to SVDAPREP.EXE are entered in the present interface and are stored in the svdaprep.dat file prior to running PEST. The *svdabatch.bat* file encapsulates necessary steps for running the model.
  3. *Run PEST*:
     PEST is executed to use the *pestctl.pst* file generated in the previous step. This PEST run will create two files, namely *pestctl.par* and *svda.bpa*. The former stores the estimated values of super parameters; the latter contains the estimated values of the base parameters.
  4. *Rename pestctl.par and svda.bpa*:
     Once the parameter estimation process is complete, the *pestctl.par* file is renamed to *pestctl._par* and *svda.bpa* is copied to *pestctl.par*. When you click on *Models* | *PEST (Parameter Estimation)* | *View* | *Estimated Parameter Values*, the *pestctl.par* file is displayed. When you click on the *Update* button of Fig. 2.82, the initial parameter values (*PARVAL1*) of the Parameters tab are updated with the values stored in *pestctl.par*.
- *Automatic calculation of first iteration super parameter derivatives*:
  If this box is cleared, super parameter derivatives calculation takes place through finite differences in the usual manner during the first optimization iteration of the inversion process. If this box is checked, PEST calculates super parameter derivatives internally for the first iteration of the SVD-assisted parameter estimation process, removing the necessity for any model runs to be undertaken in calculating these derivatives.
- *Computation of super parameters*:
  Super parameters can be calculated internally by PEST on the basis of sensitivities supplied in the Jacobian matrix (i.e., the *svda.jco* file mentioned above).Four options are available here:

  - *SVD on Q^(1/2)X*:
    This option sets SVDA_EXTSUPER to 0 in the PEST control file (i.e., the aforementioned *pestctl.pst* file). PEST will formulate super parameters through singular value decomposition of $Q^{1/2}X$, where X represents the base parameter Jacobian matrix contained in the nominated base Jacobian matrix file.
  - *SVD on XtQX*:
    This option sets SVDA_EXTSUPER to 3 in the PEST control file, which directs PEST to formulate super parameters through singular value decomposition of $XtQX$.
  - *LSQR without orthogenalization*:
    This option sets SVDA_EXTSUPER to 2 in the PEST control file, which directs PEST to calculate super parameters using the first m "v" vectors computed by the LSQR algorithm, where m is the number of super parameters (see below).
  - *LSQR with orthogonalization*:
    Same as above, however, the vectors are orthogonalized before being employed for definition of super parameters. This option sets SVDA_EXTSUPER to -2 in the PEST control file.
- *Number of super parameters to estimate*:
  Enter an appropriate number. It is sometimes wise to enter a number here which is somewhat above the expected dimensionality of estimable parameter space to accommodate shortcomings in the linearity assumption involved in determination of super parameters from base parameters. Inclusion of Tikhonov regularization in the inversion process (or use of singular value decomposition) will guarantee numerical stability of the SVD-assisted process. In either case, this number should be less (often significantly less) than the number of base estimable parameters; parameter reduction factors of up to 10 are not uncommon. Where parameters are outnumbered by observations, the number of super parameters should be at most equal to the number of observations available for model calibration. It is important to note that parameters that are fixed or tied will remain fixed and tied when defining super parameters; hence the SVD-assisted parameter estimation process will respect their status.
- *Offset for super parameters*:
  In the SVD-assisted parameter estimation process, super parameters are provided with a starting value of zero (signifying zero perturbation of initial base parameters). However zero valued parameters can create problems for PEST, especially in the enforcement of parameter change limits. Hence it is best to supply an offset for such parameters, to keep their values away from zero. A value of 10 is suitable on most occasions of SVD-assisted parameter estimation.
- *Parameter relative change limit (RELPARMAX)*:
  Base parameters are designated as "relative limited" by SVDAPREP. On most occasions a value of 0.1 will be adequate, though you should be prepared to alter this upwards if PEST convergence is too slow, or downwards if parameter oscillation occurs, or parameters hit their bounds too quickly.

- *Parameter scaling control variable (SVDA_SCALADJ)*:
  PEST provides a variety of automatic base parameter scaling mechanisms to combat the problems associated with base parameter hypersensitivity described in Section 2.8 of *Addendum to the PEST Manual* [39]. When some parameters are not log-transformed, parameter scaling is essential. Permissible values of SVDA_SCALADJ are -4, -3, -2, -1, 0, 1, 2, 3, and 4. No base parameter scaling is undertaken if SVDA_SCALADJ is set to zero.
- *Save Multiple BPA files*:
  If this box is checked, SVDA_MULBPA in the PEST control file (i.e., *pestctl.pst*) is set to 1 meaning that a series of BPA files will be recorded in the course of the parameter estimation process. Each BPA file contains base parameter values as estimated during subsequent optimization iterations (i.e., *svda.bpa.0* contains the initial base parameters; *svda.bpa.1* contains the base parameters after the first optimization iteration, and so on). In addition, a final BPA file (i.e., *svda.bpa*) will created at the end of optimization iterations. Note that not all optimization iterations will be represented in this sequence–only those iterations will be represented where base parameters are improved from those previously achieved during the current parameter estimation process.
  In normal operation, when the parameter estimation process is complete, PEST undertakes a single model run using optimized parameters before terminating execution; thus model input and output files contain best-fit parameter values and corresponding best-fit model outputs. This is not possible when undertaking SVD-assisted parameter estimation. However, based on the contents of the *svda.bpa* file (which is copied to *PESTCTL.PAR* by **PM** at the end of the parameter estimation process), the user can carry out such a model run by simply clicking on the *Update* button to import the estimated base parameter values from *PESTCTL.PAR* to the Parameter tab, set *Operation Mode* (Fig. 2.82) to *Forward Model Run using PARVAL values given in the Parameters tab*, and then run PEST.
- *Save Multiple JCO files*:
  If this box is checked, PEST will write a Jacobian matrix file (i.e., a "JCO file") at the end of each optimization iteration, this containing the Jacobian matrix employed for that particular iteration.
- *Save Multiple REI files*:
  If this box is checked, PEST will write a residuals file (i.e., a "REI file") at the end of each optimization iteration.

The Control Data Tab

The control data are used to set internal array dimensions of PEST and tune the optimization algorithm to the problem at hand. The items of the Control Data tab (Fig. 2.83) are described in detail below. When in doubt, the user should use the default values.

- *RLAMBDA1* is the initial Marquardt lambda. PEST attempts parameter improvement using a number of different Marquardt lambdas during any optimization it-

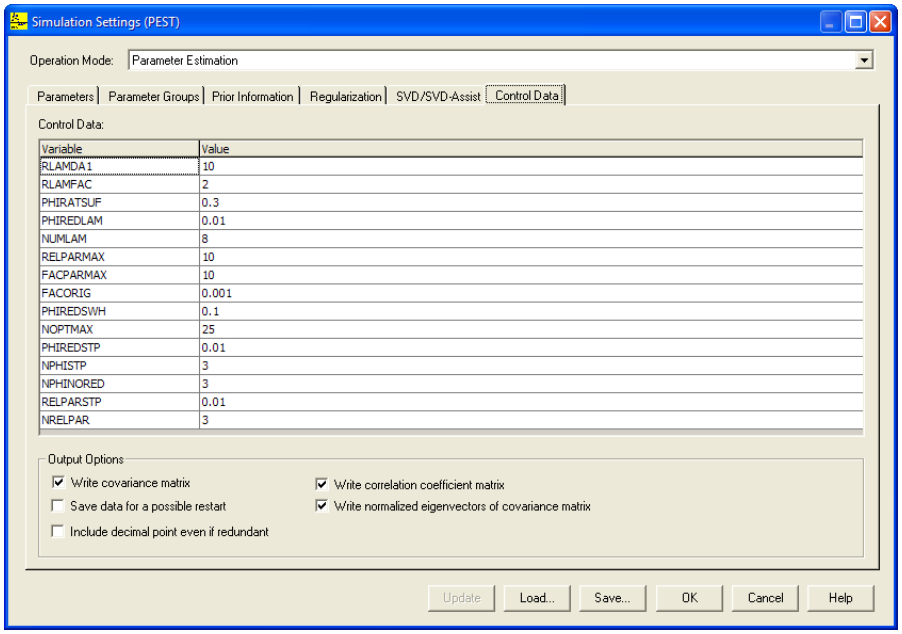


Fig. 2.83. The Control Data tab of the Simulation Settings (PEST) dialog box

eration. In the course of the overall parameter estimation process, the Marquardt lambda generally gets smaller. An initial value of 1.0 to 10.0 is appropriate for many models, though if PEST complains that the normal matrix is not positive definite, you will need to provide a higher initial Marquardt lambda. For high values of the Marquardt parameter (and hence of the Marquardt lambda) the parameter estimation process approximates the gradient method of optimization. While the latter method is inefficient and slow if used for the entire optimization process, it often helps in getting the process started, especially if initial parameter estimates are poor. PEST reduces lambda if it can. However if the normal matrix is not positive definite or if a reduction in lambda does not lower the objective function, PEST has no choice but to increase lambda.

- *RLAMFAC* is the factor by which the Marquardt lambda is adjusted. RLAMFAC must be greater than 1.0. When PEST reduces lambda it divides by RLAMFAC; when it increases lambda it multiplies by RLAMFAC.
- *PHIRATSUF* is the first criterion for moving to the next optimization iteration. During any optimization iteration, PEST tries lots of parameter sets and will consider that the goal of the iteration has been achieved if

$$\frac{\phi_i}{\phi_{i-1}} \leq PHIRATSUF \tag{2.61}$$

where ϕ_{i-1} is the lowest objective function calculated for optimization iteration i-1 (and hence the starting value for the i-th optimization iteration) and ϕ_i is the

objective function corresponding to a parameter set during optimization iteration i.

A value of 0.3 is often appropriate for PHIRATSUF. If it is set too low, model runs may be wasted in search of an objective function reduction, which it is not possible to achieve. If it is set too high, PEST may not be given the opportunity of refining lambda in order that its value continues to be optimal as the parameter estimation process progresses.

- *NUMLAM* is the maximum number of lambdas (parameter sets) that PEST can test during any optimization iteration. It should normally be set between 5 and 10. For cases where parameters are being adjusted near their upper or lower limits, and for which some parameters are consequently being frozen (thus reducing the dimension of the problem in parameter space) experience has shown that a value closer to 10 may be more appropriate than one closer to 5.
- *RELPARMAX* and *FACPARMAX* are used to limit parameter adjustments. RELPARMAX is the maximum relative change that a parameter is allowed to undergo between iterations, whereas FACPARMAX is the maximum factor change that a parameter is allowed to undergo. A parameter is denoted as either relative limited or factor limited through PARCHGLIM (see page 154).
  - If a parameter b is relative limited, the relative change of the parameter value between optimization iterations i-1 and i is defined as

$$\frac{(b_{i-1} - b_i)}{b_{i-1}} \tag{2.62}$$

    The absolute value of this relative change must be less than RELPARMAX. If a parameter upgrade vector is calculated such that the relative adjustment for one or more relative limited parameters is greater than RELPARMAX, the magnitude of the upgrade vector is reduced such that this no longer occurs.
  - If parameter b is factor limited, the factor change between optimization iterations i-1 and i is defined as

$$\begin{array}{ll} b_{i-1}/b_i & \text{if} \quad |b_{i-1}| > |b_i| \\ b_i/b_{i-1} & \text{if} \quad |b_{i-1}| \leq |b_i| \end{array} \tag{2.63}$$

    This factor change must be less than FACPARMAX. If a parameter upgrade vector is calculated such that the factor adjustment for one or more factor limited parameters is greater than FACPARMAX, the magnitude of the upgrade vector is reduced such that this no longer occurs.

It is important to note that a factor-limit will not allow a parameter to change sign. If a parameter must be free to change sign during an optimization process, it must be relative limited; furthermore RELPARMAX must be set at greater than unity or the change of sign will be impossible. Similarly, if a parameter's upper or lower limit is zero, it cannot be factor limited and RELPARMAX must be at least unity.

Suitable values for RELPARMAX and FACPARMAX can vary enormously from case to case. If you are unsure of how to set these parameters, a value of 5 for

each of them is often suitable. For highly non linear problems, these values are best set low. If they are set too low, however, the estimation process can be very slow. An inspection of the PEST run record (by pressing the ESC key) will often show whether you have set these values too low, for PEST records the maximum parameter factor and relative changes are recorded on this file at the end of each optimization iteration. If these changes are always at their upper limits and the estimation process is showing no signs of instability, it is quite possible that RELPARMAX and/or FACPARMAX are too low and could be increased.
Note that FACPARMAX can never be less than 1; RELPARMAX can be less than 1 as long as no parameter's upper and lower bounds are of opposite sign. (If necessary, use OFFSET to shift the parameter domain so that it does not include zero.)

- *FACORIG* is a criterion for modifying RELPARMAX and FACPARMAX. If, in the course of an estimation process, the absolute value of a parameter falls below the product of FACORIG and its original value, then the product is substituted for the denominators of equation 2.62 or equation 2.63 to prevent the denominators becoming zero or too small. FACORIG is not used to adjust limits for log transformed parameters. FACORIG must be greater than zero. A value of 0.001 is often adequate.
- *PHIREDSWH* is a criterion for switching the calculation method of derivatives between the forward finite difference method and the central finite difference method. If, for the i-th iteration the relative reduction in the objective function between successive optimization iterations is less than PHIREDSWH, PEST will switch to three point derivatives calculation for those parameter groups with FORCEN = Switch. The relative reduction in the objective function is defined by $[(\phi_{i-1} - \phi_i)/\phi_{i-1}]$, where ϕ_i is the objective function calculated on the basis of the upgraded parameter set determined in the i-th iteration.
  A value of 0.1 is often suitable for PHIREDSWH. If it is set too high, PEST may make the switch to three point derivatives calculation too early. The result will be that more model runs will be required than are really needed at that stage of the estimation process. If PHIREDSWH is set too low, PEST may waste an optimization iteration or two in lowering the objective function to a smaller extent than would have been possible, if it had made an earlier switch to central derivatives calculation.
  Note that PHIREDSWH should be set considerably higher than PHIREDSTP (see below) which sets one of the termination criteria on the ba-sis of the relative objective function reduction between optimization iterations.
- *NOPTMAX* is the maximum number of optimization iterations. A value of 20 to 30 is often adequate. If you want to ensure that PEST termination is triggered by other criteria, more indicative of parameter convergence to an optimal set or of the futility of further processing, you should set this variable very high.
- *PHIREDSTP* and *NPHISTP* are convergence criteria. For many cases 0.01 and 3 are suitable values for PHIREDSTP and NPHISTP respectively. If, in the course of the parameter estimation process, there have been NPHISTP optimization iterations for which

$$\frac{(\phi_i - \phi_{min})}{\phi_i} \leq PHIREDSTP \tag{2.64}$$

(ϕ_i being the objective function value at the end of the i-th optimization iteration and ϕ_{min} being the lowest objective function achieved to date), PEST will end the optimization process.

- *NPHINORED* is the first termination criterion. A value of 3 is often suitable. If PEST has failed to lower the objective function over NPHINORED successive iterations, the program stops.
- *RELPARSTP* and *NRELPAR* represent the second termination criterion. If the magnitude of the maximum relative parameter change between optimization iterations is less than RELPARSTP over NRELPAR successive iterations, the program stops. The relative parameter change between optimization iterations for any parameter is calculated using equation 3.55. For many cases, a value of 0.01 for RELPARSTP and a value of 3 for NRELPAR are adequate.
- *Output Options* When the optimization process is complete, one of the termination criteria having been met (or perhaps another termination criterion such as zero objective function or zero objective function gradient, for which no user supplied settings are required), PEST writes some information concerning the optimized parameter set to its run record file PESTCTL.REC. This file is saved in the data directory of your model. It tabulates the optimal values and the 95% confidence intervals pertaining to all adjustable parameters. It also tabulates the model calculated values based on these parameters, together with the residuals, i.e., the differences between measured and model calculated values.
  - *Write covariance matrix*: If checked, PEST will write the parameter covariance matrix to the run record file PESTCTL.REC.
  - *Write correlation coefficient matrix*: If checked, PEST will write the parameter correlation coefficient matrix to the run record file PESTCTL.REC.
  - *Write normalized eigenvectors of covariance matrix*: If checked, PEST will write the normalized eigenvectors of the covariance matrix to the run record file PESTCTL.REC.
  - *Save data for a possible restart*: If checked, PEST will dump the contents of many of its data arrays to a binary file at the beginning of each optimization iteration; this allows PEST to be restarted later if execution is prematurely terminated. If subsequent PEST execution is initiated using the "/r" command line switch (see the PEST manual[34] for details), it will recommence execution at the beginning of the iteration during which it was interrupted.
  - *Include decimal point even if redundant*: If cleared, PEST will omit the decimal point from parameter values on model input files if the decimal point is redundant, thus making room for the use of one extra significant figure. If this option is checked, PEST will ensure that the decimal point is always present.

2.6.8.2 PEST (Parameter Estimation) | Head Observations

Select the Head Observations from the *PEST (Parameter Estimation)* menu (or from *MODFLOW*, *MODFLOW-2000 (Parameter Estimation)*) to specify the locations of

the head observation boreholes and their associated observed (measurement) data in a Head Observation dialog box. See Section 2.6.1.14 for details.

When this menu item is selected (and checked), PEST uses the head observation data for the parameter estimation.

2.6.8.3 PEST (Parameter Estimation) | Flow Observations

Select Drawdown Observations from the *PEST (Parameter Estimation)* or *MODFLOW* menu to specify the locations of the drawdown observation boreholes and their associated observed (measurement) data in a Drawdown Observations dialog box. Its use is identical to the Head Observation dialog box. The only difference is that the head observations are replaced by drawdown observations. See Section 2.6.1.14 for details.

When this menu item is selected (and checked), PEST uses the drawdown observation data for the parameter estimation.

2.6.8.4 PEST (Parameter Estimation) | Run

Select this menu item to start a parameter estimation (model calibration) process with PEST. The available settings of the Run PEST dialog box (Fig. 2.84) are described below.

- The File Table has three columns:
  - *Generate*: **PM** uses the user-specified data to generate input files for MODFLOW and PEST. An input file will be generated if it does not exist or if

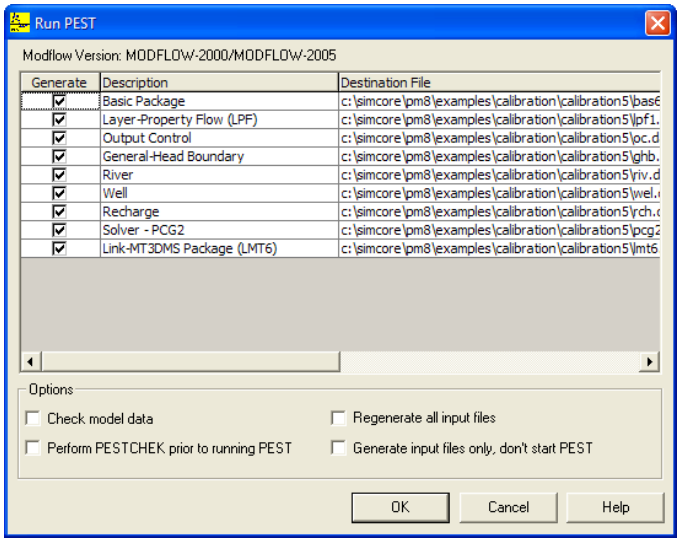


Fig. 2.84. The Run PEST dialog box

the corresponding *Generate* box is checked. The user may click on a box to check or clear it. Normally, we do not need to worry about these boxes since **PM** will take care of the settings.
  - *Description* gives the names of the packages used in the model.
  - *Destination File* shows the paths and names of the input files of the model.
- Options:
  - *Regenerate all input files*: Check this option to force **PM** to generate all input files regardless the setting of the Generate boxes. This is useful if the input files have been deleted or overwritten by other programs.
  - *Generate input files only, don't start PEST*: Check this option, if the user does not want to run PEST. The program can be started at a later time or can be started at the Command Prompt (DOS box) by executing the batch file PEST.BAT.
  - Perform PESTCHEK prior to running PEST: PESTCHEK reads the PEST input files generated by **PM**, making sure that every item is consistent with every other item and writes errors to the file PEST.CHK. It is recommended to use PESTCHEK, as **PM** and PEST do not carry out consistency checks of all user-specified control data and parameters.
  - *Check the model data*: If this option is checked, **PM** will check the geometry of the model and the consistency of the model data as given in Table 2.6 before creating data files. The errors (if any) are saved in the file CHECK.LIS located in the same folder as the model data.
- *OK*: Click *OK* to generate MODFLOW and PEST input files. In addition to the input files, **PM** creates a batch files PEST.BAT and MODELRUN.BAT in the model folder. When all files are generated, **PM** automatically runs PEST.BAT in a Command Prompt-window (DOS box). PEST.BAT will call the other batch file MODELRUN.BAT. During a parameter estimation process, PEST prints the estimated parameter values to the run record file PESTCTL.REC in the model folder and writes the estimated parameter values to the corresponding input files of MODFLOW (BCF.DAT, WEL.DAT,... , etc.). So, after a parameter process, the simulation results of MODFLOW are updated by using the most recently estimated parameter values. PEST does not modify the original model data. This provides a greater security to the model data since a parameter estimation process does not necessarily lead to a success.

2.6.8.5 PEST (Parameter Estimation) | View

PEST (Parameter Estimation) | View | Run Record File

Select this menu item to use the Text Viewer (see Section 2.3.4) to display the run record file PESTCTL.REC, which contains the optimized value of each adjustable parameter together with that parameter's 95% confidence interval. It tabulates the set of field measurements, their optimized model-calculated counterparts, the difference between each pair, and certain functions of these differences.

PEST (Parameter Estimation) | View | Forward Run Listing File

During a parameter estimation process, forward runs are repeated and the run record is saved in the listing file OUTPUT.DAT. Listing files are overwritten during subsequent forward model runs and thus only the listing file unique to final parameter values is available for inspection with the Text Viewer (see Section 2.3.4).

Parameter estimation processes are often terminated unexpectedly because MODFLOW fails to complete a flow calculation due to an unsuitable parameter combination used by an estimation-iteration. In that case, MODFLOW writes error messages to the listing file OUTPUT.DAT and terminates the simulation. It is therefore recommended to check this file when PEST fails to complete the parameter estimation iterations.

PEST (Parameter Estimation) | View | Estimated Parameter Values

At the end of each optimization-iteration, PEST writes the best parameter set achieved so far (i.e., the set for which the objective function is lowest) to a file named PESTCTL.PAR. Select this menu item to use the Text Viewer (see Section 2.3.4) to display this file. The first line of the PESTCTL.PAR file contains the values for the character variables PRECIS and DPOINT, which were used in the PEST control file. Then follows a line for each parameter, each line containing a parameter name, its current value and the values of the SCALE and OFFSET variables for that parameter. Refer to Doherty [34] for details about PRECIS, DPOINT, SCALE and OFFSET.

Using values from intermediate parameter-estimation iterations, that are likely to be closer to the optimal parameter values, often reduces execution time.

PEST (Parameter Estimation) | View | Composite Parameter Sensitivities

Select this menu item to use the Text Viewer (see Section 2.3.4) to display the Parameter Sensitivity file PESTCTL.SEN, which contains composite parameter sensitivity values. The composite sensitivity of a parameter is defined in Equation (5.1) of the PEST manual [34]. As given in the PEST manual, composite parameter sensitivities are useful in identifying those parameters which may be degrading the performance of the parameter estimation process through lack of sensitivity to model outcomes.

PEST (Parameter Estimation) | View | Composite Observation Sensitivities

Select this menu item to use the Text Viewer (see Section 2.3.4) to display the Observation Sensitivity file PESTCTL.SEO, which contains all observation values and corresponding model-calculated values, as well as composite sensitivities for all observations. The composite sensitivity of an observation is a measure of the sensitivity of that observation to all parameters involved in the parameter estimation process. A high value of composite observation sensitivity normally indicates that an observation is particularly crucial to the inversion process. Refer to Section 5.1.6 of the PEST manual [34] for more details.

PEST (Parameter Estimation) | View | Head Scatter Diagram

This menu item is available only if Head Observations have been defined (see Section 2.6.1.14). Select this menu item to open a Scatter Diagram (Hydraulic Head) dialog box. Refer to Section 2.6.1.20 for details.

PEST (Parameter Estimation) | View | Drawdown Scatter Diagram

This menu item is available only if Drawdown Observations have been defined (see Section 2.6.1.15). Select this menu item to open a Scatter Diagram (Drawdown) dialog box, which is identical to the Scatter Diagram (Hydraulic Head) dialog box,

except the drawdown values replace the head values. Refer to Section 2.6.1.20 for details.

PEST (Parameter Estimation) | View | Head-Time Curves

This menu item is available only if Head Observations have been defined (see Section 2.6.1.14). Select this menu item to open a Time Series Curves (Hydraulic Head) dialog box. Refer to Section 2.6.1.20 for details.

PEST (Parameter Estimation) | View | Drawdown-Time Curves

This menu item is available only if Drawdown Observations have been defined (see Section 2.6.1.15). Select this menu item to open a Time Series Curves (Drawdown) dialog box, which is identical to the Time Series Curves (Hydraulic Head) dialog box, except the drawdown values replace the head values. Refer to Section 2.6.1.20 for details.

2.6.9 PMPATH (Advective Transport)

Select this menu to call the particle-tracking model PMPATH, which runs independently from **PM**. Refer to Chapter 3 for details.

Note. PMPATH can be started by selecting this menu or from the Start menu of Windows. When PMPATH is started from **PM**, it will automatically load the model currently used by **PM**. If the model data have been subsequently modified and a flow simulation has been performed, the modified model must be re-loaded into PMPATH to ensure that it can recognize the modifications.

2.7 The Tools Menu

2.7.1 Digitizer

The Digitizer is based on the Data Editor. Using the Digitizer the user can digitize, shift or delete points, and assign values to the points. The menu item Points in the Value menu allows the user to save, delete, or load points. **PM** saves or loads points to/from XYZ files. An XYZ file stores the number of points, the (x, y) coordinates, and the associated values of all points. Refer to Section 6.2.10 for the format.

► To digitize a point

1. Click the Digitize button .
   It is not necessary to click the button if it is already depressed.
2. Click the mouse pointer on the desired position to set a point.

► To shift a digitized point

1. Click the Digitize button .
2. Point the mouse pointer to a digitized point, left-click and hold down the mouse button, and then move the mouse to drag the digitized point.
3. Release the mouse button when the point is moved to the desired position.

► To delete a digitized point

1. Click the Digitize button .
2. Hold down the Ctrl key and left-click on the point to be deleted.

► To assign a value to a digitized point

1. Click the Digitize button .
2. Move the mouse pointer to the point to be assigned a value.
3. Right-click on the point.
   The Digitizer shows a dialog box.
4. In the dialog box, type a new value then click OK.

2.7.2 The Field Interpolator

2.7.2.1 Interpolation Methods for Irregularly Spaced Data

Numerical groundwater models require parameters (e.g. hydraulic conductivity, hydraulic heads, elevations of geological layers etc.) assigned to each model cell. Hydrogeologists, however, often obtain a parameter distribution in the form of scattered (irregular) data points (x_i, y_i, f_i), i = 1, ..., N. N is the number of measurement points, x_i and y_i are the coordinates and f_i is the parameter value at point i. A fundamental problem is how to estimate the parameter values for each model cell from these data.

A number of interpolation (or extrapolation) methods for solving this kind of problems do exist. Some of the methods are used by commercial contouring software, e.g. GEOKRIG, GRIDZO, SURFER, or TECKONEM. Some implementations are published and available at no cost, e.g., GSLIB [31]. In an earlier time, a common approach used by many modelers is that contour maps are first created either by using software packages or manually then overlaid on the model grid for assigning parameter values to model cells. The process is indirect and somewhat cumbersome.

The Field Interpolator provides a more direct way for assigning cell values by using the Kriging method and methods developed by Shepard [108], Akima [1][2], and Renka [100][101]. The programs interpolate or extrapolate the measurement data to each model cell. The model grid can be irregularly spaced. Interpolation results are saved in the ASCII Matrix format (see Section 6.2.1), which can be imported by the Data Editor into the model grid. Depending on the interpolation method and the interpolation parameters the results may be different. Using the Data Editor, the user may create contour maps of the interpolation results and visually choose a ”best” one.

Theory is not emphasized in this description since it is introduced in extensive literature. For example, Watson [113] presents a guide to the analysis and display of spatial data, including several interpolation methods. Franke [45] provides a brief review and classification of 32 algorithms. Hoschek and Lasser [64] give a comprehensive discussion of theories in geometrical data processing and extensive references in the area of data interpolation and computer graphics techniques. Akin and Siemes [3] and Davis [30] provide fundamental mathematical background on the statistics and data analysis in geology.

2.7.2.2 Using the Field Interpolator

The Field Interpolator runs independently from **PM**. To start the program, select *Tools* | *Field Interpolator* from **PM** or select *Field Interpolator* from the *Start* menu of Windows. The settings of the Field Interpolator (Fig. 2.85) are grouped under three tabs - Files, Grid Position and Search/Gridding Method. These tabs are described below. To start the interpolation, simply click the *GO* button. The Field Generator creates and writes the settings and the coordinates to a batch file PMDIS.BAT and two ASCII files PMDIS_IN.{1} and PMDIS_IN.{2}. After having created these files, PMDIS.BAT starts in a DOS-window. The created ASCII files are used by the interpolation program.

The Files Tab

- *PMWIN Model*: If the user has already opened a model within **PM** and started the Field Interpolator from the Tools menu, this field contains the model file name. If the text string "Open a model first" is shown, click and select a **PM** model from an Open File dialog box. A **PM** model file always has the extension .PM5.
- *Input File*: An input file contains the measurement data, which are saved as an XYZ file (see Section 6.2.10 for the format). An input file can be prepared with the Digitizer or other software. Click to select an existing input file. The maximum number of data points is 5000.

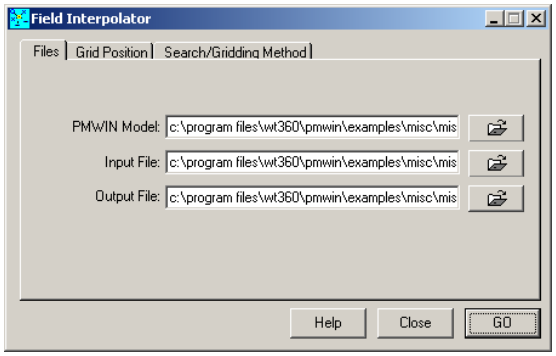


Fig. 2.85. The Field Interpolator dialog box

- Output file: An output file contains the interpolated data for each model cell and is saved in the ASCII matrix format. See Section 6.2.1 for the format of the ASCII matrix file.

The Grid Position Tab

Using the rotation angle and the coordinates (Xo, Yo) of the upper-left corner of the model grid, the user may rotate and place the grid at any position. The rotation angle is expressed in degrees and is measured counterclockwise from the positive x-direction. See Section 2.9.2 for details about the coordinate system of **PM**. As we normally define the grid position and the coordinate system at the beginning of a modeling process, the grid position will rarely need to be changed here.

The Gridding Method Tab

PMWIN provides four gridding methods. The user may select a method from the drop-down box. There is a corresponding interpolation program for each gridding method. The interpolation programs are written in FORTRAN and were compiled with the Lahey FORTRAN 95 compiler. The following sections give details of the gridding (or interpolation) methods.

- *Shepard's Inverse Distance*: The Shepard's inverse distance method uses Equation 2.65 to interpolate data for finite-difference cells.

$$f = \frac{\sum_{i=1}^{N} \left[f_i / d_i^F \right]}{\sum_{i=1}^{N} \left[1 / d_i^F \right]} \tag{2.65}$$

  Where d_i is the distance between data point i and the center of a model cell, f_i is the value at the i-th data point, F is the weighting exponent and f is the estimated value at the model cell.
  The weighting exponent must be greater than zero and less than or equal to 10. Fig. 2.86 shows the effects of different weighting exponents. Five data points are regularly distributed along the x-axis. Using higher values for the exponent (e.g., F = 4) the interpolated cell values will approach the value of the nearest data point. The surface is therefore relatively flat near all data points. Lower values of the exponent (e.g. F = 1) produce a surface with peaks to attain the proper values at the data points. A value of F = 2 is suggested by Shepard [108].
- *Akima's bivariate interpolation*: This method creates a triangulation of the measurement data points and performs interpolation by using a bivariate fifth order Hermite polynomial for the interpolation within a triangle. It uses a user-specified number of data points closest to a model cell for estimating the value at the cell.

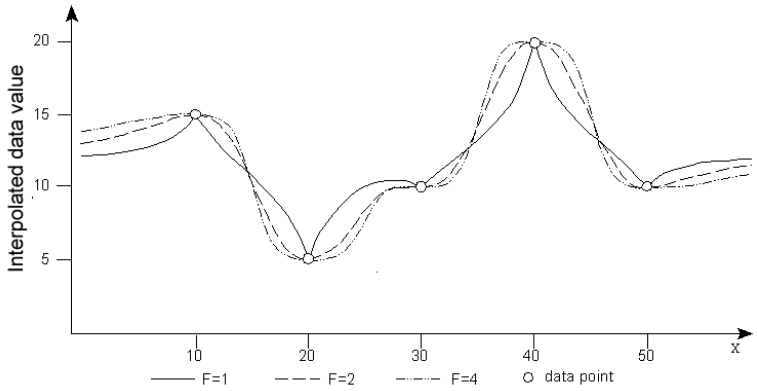


Fig. 2.86. Effects of different weighting exponents

- *Renka's triangulation*: This method first creates a triangulation of the measurement data points and then uses a global derivative-estimation procedure to compute estimated partial derivatives at each point. The program determines a piecewise cubic function F(x,y). F has continuous first derivatives over the created mesh and extends beyond the mesh boundary allowing extrapolation.
- *Kriging*: The Kriging method has been popularized by Mathéron [84] and is named in honor of D. G. Krige, a noted South African mining geologist and statistician. **PM** assumes that the measurement data are stationary and isotropic. The Kriging method estimates the value at a model cell from a user-specified number of adjacent data values while considering the interdependence expressed in the variogram.
  A variogram is a plot of semivariance $\gamma_{(h)}$ versus vector distance h. The variogram is used to define the relationship of the measurement values or to estimate the distance over which measurement values are interdependent. When Kriging is selected as the gridding method, a Variogram button appears. Click this button to display the Variogram dialog box (Fig. 2.87). The user needs to select a variogram model from the drop-down box and specify the parameters for the selected variogram model. **PM** does not provide a procedure for fitting the selected variogram curve to the measurement data. This is a task for geostatistical software, e.g., VarioWin [92] or GEO-EAS [42], and beyond the objective of this software. Consider other interpolation methods, if the variogram type is unknown.

  The meaning of necessary parameters and the equations for the variogram models are listed below:
  – Power and linear model:

$$\gamma_{(h)} = \alpha \cdot |h|^{\omega} + c_0 \qquad \alpha > 0 \text{ and } 0 < \omega < 2 \qquad (2.66)$$

  – Logarithmic model:

$$\gamma_{(h)} = 3 \cdot \alpha \cdot log|h| + c_0 \qquad \alpha > 0 \qquad (2.67)$$

– Spherical model:

$$\gamma_{(h)} = C \cdot \left(\frac{3}{2} \cdot \frac{|h|}{a} - \frac{|h|^3}{2 \cdot a^3} \right) + c_0 \qquad h \leq a$$
$$\gamma_{(h)} = C + c_0 \qquad h > a \qquad (2.68)$$

– Gaussian model:

$$\gamma_{(h)} = C \cdot \left[1 - EXP\left(-\frac{h^2}{a^2} \right) \right] + c_o \qquad (2.69)$$

– Exponential model:

$$\gamma_{(h)} = C \cdot \left[1 - EXP\left(-\frac{|h|}{a} \right) \right] + c_o \qquad (2.70)$$

Where C is the variance of measurement data and is calculated by the program, a is the correlation length, c_0 the nugget variance, α the slope and ω the power factor of the power model. ω = 1 yields the linear model (Fig. 2.88).

The Search Method Tab

The interpolation algorithms use three search methods to find a certain number of the measurement data points to interpolate a cell value. The search methods are called SIMPLE, QUADRANT and OCTANT. The search radius is assumed to be infinitely large.

The SIMPLE search method finds the data points nearest to the model cell. The QUADRANT or OCTANT search methods find closest data points from each quadrant or octant around a model cell (Figures 2.89a and 2.89b). The number of data points used in a search is defined by the *Data Per Sector* value. If fewer than *Data*

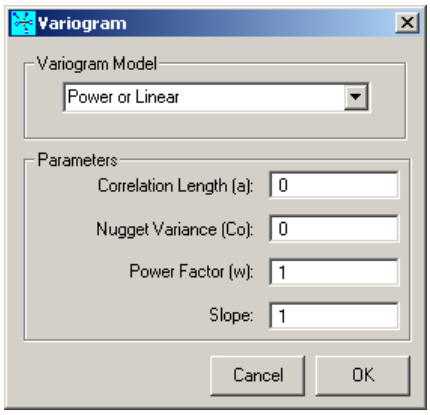


Fig. 2.87. The Variogram dialog box

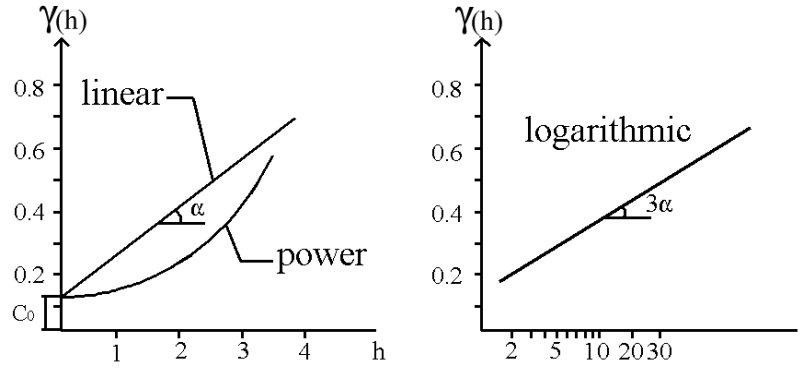


Fig. 2.88. Linear, Power and logarithmic models

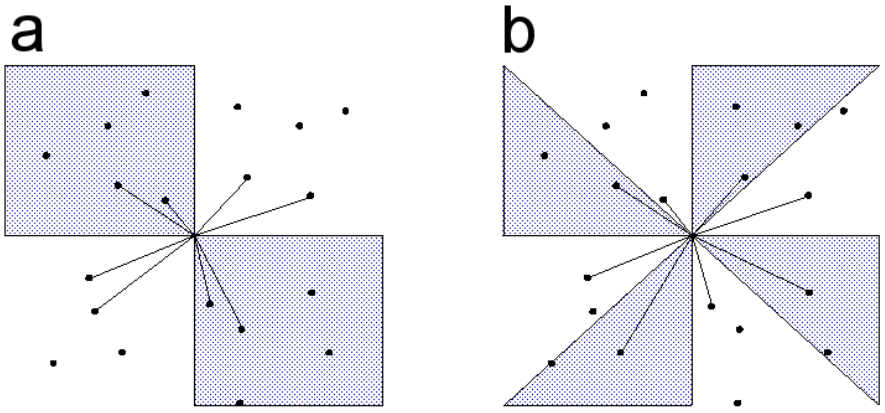


Fig. 2.89. Search patterns used by (a) the Quadrant Search method (Data per sector=2) and (b) the Octant Search method (Data per sector=1)

Per Sector points are found in a sector, the program uses the other nearest points found in the entire model. The valid range of *Data Per Sector* is

SIMPLE:	$3 \leq Data\ Per\ Sector \leq 30$
QUADRANT:	$1 \leq Data\ Per\ Sector \leq 7$
OCTANT:	$1 \leq Data\ Per\ Sector \leq 3$

The search method defaults to OCTANT search. Octant or quadrant searches are usually used when the measurement points are grouped in clusters. These search methods force the interpolation programs to use measurement data points radially distributed around the model cell. They usually introduce more smoothing than a SIMPLE search.

Note that the entries in Search Method are ignored when Renka's triangulation algorithm is used.

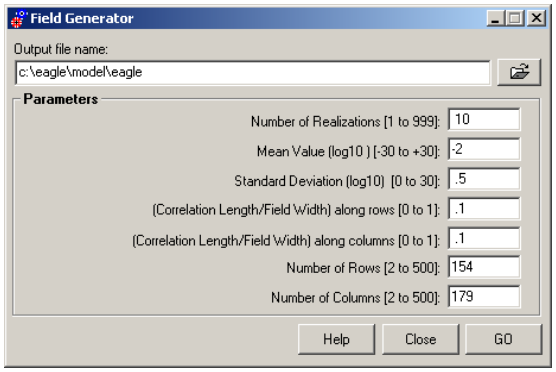


Fig. 2.90. The Field Generator dialog box

2.7.3 The Field Generator

The Field Generator (Frenzel [47]) can generate fields with heterogeneously distributed transmissivity or hydraulic conductivity values. This allows the user to perform stochastic modeling by considering parameter distributions within **PM**. In stochastic modeling, uncertainty due to unknown spatial variability of the model parameters is addressed directly by assuming that the parameters are random variables. Hydraulic conductivity or transmissivity is commonly assumed to be lognormally distributed. We denote the hydraulic conductivity by X and define a variable $Y = log(X)$. When Y is normally distributed with a mean value μ and standard deviation σ, then X has a log-normal distribution.

The Field Generator runs independently from **PM**. To start the program, select *Tools* | *Field Generator* from **PM** or select *Field Generator* from the *Start* menu of Windows. The program displays one dialog box (Fig. 2.90) and is fairly easy to use. It uses the correlation scales in both I (row) and J (column) directions and the mean value μ and standard deviation σ of log-transformed measurement values to generate a quantitative description (a realization) of the hydraulic conductivity or transmissivity field. The size of the field (number of cells) and the number of desired realizations are specified in the dialog box. Realizations are saved in the ASCII Matrix format (see Section 6.2.1) using the file names *filename.nnn*, where *filename* is the output file name specified in the dialog and *nnn* is the realization number. Note that *filename* must not be the same as the name of the model.

The generated field is log-normally (to base 10) distributed. Using the Data Editor, the user can load the generated field into an area of the model grid where the columns and rows are regularly spaced (see Section 2.8.1 for how to load an ASCII matrix file). The simulation of the hydraulic conductivity distribution produced in this way is not constrained to match the measurement values. In a constrained simulation existing measurements are used which reduce the space of possible realizations. A constrained simulation of a single realization proceeds in five steps:

1. The parameter value for each model cell is interpolated from the measurements using the Kriging method. The correlation length is determined from the measurements.
2. An unconstrained generation is performed using the Field Generator with the same correlation length (correlation scale).
3. The unconstrained generated values at the measurement locations are used to interpolate values for each model cell by using the Kriging method again.
4. The distribution from step 3 is subtracted from the distribution from step 2 yielding kriging-residuals.
5. The Kriging-residuals are added to the distribution from step 1 yielding a realization, which has the same correlation length and passes through the measured values at the measurement points.

2.7.4 2D Visualization

The 2D Visualization tool is based on the Data Editor and displays the contours of a selected model result type on the model grid (Fig. 2.91). The simulation result type is selected by using the Result Selection dialog box (Fig. 2.92), which is displayed after selecting the menu item *Tools | 2D Visualization*. The dialog box contains several tabs; each corresponds to a simulation model. Use these tabs to select the desired result type, and click the OK button to proceed to the 2D Visualization tool. The 2D Visualization tool will load the selected model result and automatically display 11 contour levels ranging from the minimum to maximum values. For a time-dependent result type, the user can select a time point from the Simulation Time drop-down box on the tool bar.

2.7.5 3D Visualization

Select this menu item to start the 3D Visualization program defined in the Preferences dialog box (see Section 2.3.4 for details). Currently, **PM** is supported by two 3D visualization software packages - 3D Groundwater Explorer [21] and 3D Master [23].

2.7.6 Results Extractor

Normally, simulation results from MODFLOW, MT3DMS, and other transport models are saved in unformatted (binary) files and cannot be examined by using usual text editors. Using the Results Extractor, the user may extract specific results from the result files and save them in ASCII Matrix (see Section 6.2.1 for the format) or Surfer Data files. The Result Extractor dialog box (Fig. 2.93) is described below.

- *Spreadsheet*: The spreadsheet displays a series of columns and rows, which correspond to the columns and rows of the finite-difference grid. By clicking the Read button, the selected result type will be read and put into the spread-sheet.

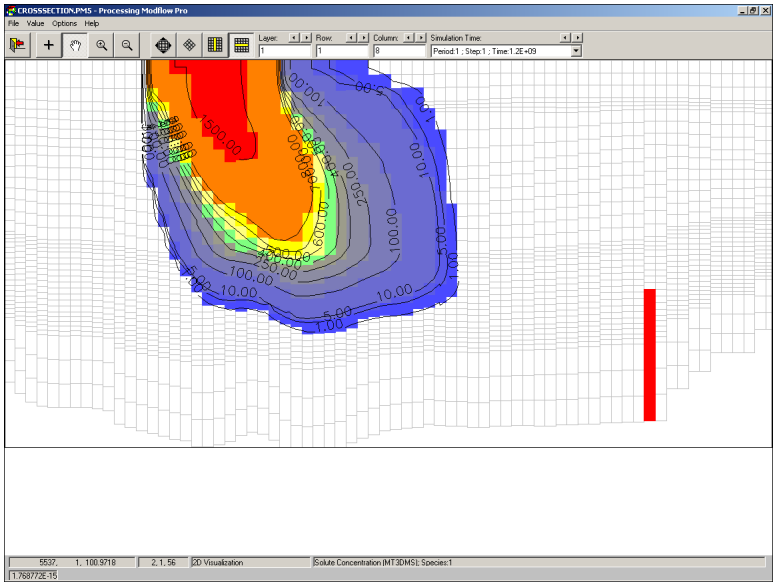


Fig. 2.91. The 2D Visualization tool in action

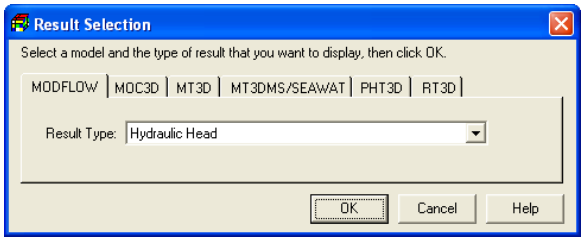
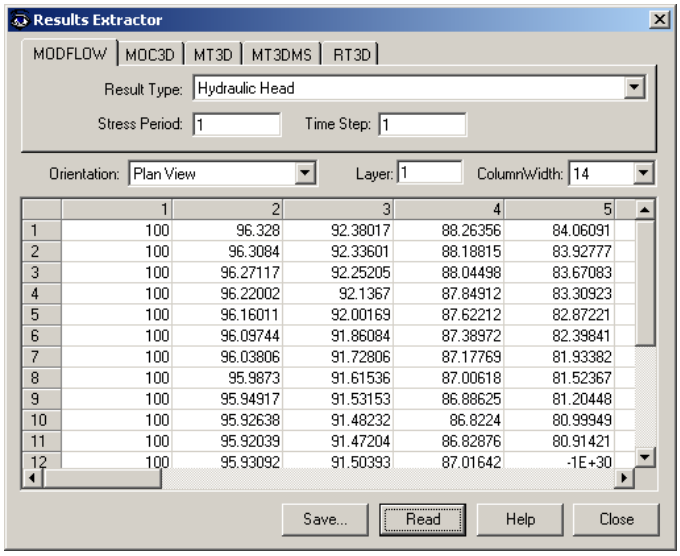


Fig. 2.92. The Result Selection dialog box

- *Orientation* and *Layer*: Simulation results can be loaded layer-, column- or row-wise. Orientation decides how the results should be loaded. If Orientation is Plan View, the user is asked to enter a layer number into the edit field. If X-section (column) or X-section (row) is selected, the user should enter a column or row number into the edit field next to drop-down box.
- *Column Width*: This drop-down box is used to change the appearance width of the columns of the spreadsheet.
- *Tabs*: Each tab corresponds to a simulation model.
  - *MODFLOW*: The available Result Types include hydraulic head, drawdown, preconsolidation head, compaction, subsidence and cell-by-cell flow terms (see Section 2.6.1.18 for the definition of each term). The stress period and time step, from which the result is read, are given in the corresponding edit fields.

  - *MOC3D*: The available Result Types are concentration and velocity terms. The simulation time, from which the result is read, can be selected from the Total Elapsed Time drop-down box. This drop-down box is empty, if the selected simulation result does not exist.
  - *MT3D*: The primary result of MT3D is concentration. When using MT3D96, two additional result types, i.e. solute mass and sorbed mass, can be selected. The simulation time, from which the result is read, can be selected from the Total Elapsed Time drop-down box. This drop-down box is empty, if the selected simulation result does not exist.
  - *MT3DMS*: The primary result of MT3DMS is concentration. When using MT3D99 [122], two additional result types, i.e. solute mass and sorbed mass, can be selected. The species number and simulation time, from which the result is read, can be selected from the Species Number and Total Elapsed Time drop-down boxes. These drop-down boxes are empty, if simulation results do not exist.
  - *RT3D*: The primary result of RT3D is concentration. The species number and simulation time, from which the result is read, can be selected from the Species Number and Total Elapsed Time drop-down boxes. These drop-down boxes are empty, if simulation results do not exist.
- *Save* and *Read*: To extract a certain result type, simply click the Read button. The spreadsheet is saved by clicking the Save button and specifying the file name and the file type in a Save Matrix As dialog box. There are four file types, ASCII Matrix (Warp form), ASCII Matrix, SURFER files and SURFER files (real-world). An ASCII Matrix file may be loaded into the model by the Data Editor at a later time. The format of the ASCII matrix file is described in Section 6.2.1. A



	1	2	3	4	5
1	100	96.328	92.38017	88.26356	84.06091
2	100	96.3084	92.33601	88.18815	83.92777
3	100	96.27117	92.25205	88.04498	83.67083
4	100	96.22002	92.1367	87.84912	83.30923
5	100	96.16011	92.00169	87.62212	82.87221
6	100	96.09744	91.86084	87.38972	82.39841
7	100	96.03806	91.72806	87.17769	81.93382
8	100	95.9873	91.61536	87.00618	81.52367
9	100	95.94917	91.53153	86.88625	81.20448
10	100	95.92638	91.48232	86.8224	80.99949
11	100	95.92039	91.47204	86.82876	80.91421
12	100	95.93092	91.50393	87.01642	-1E+30

Fig. 2.93. The Results Extractor dialog box

SURFER file has three columns containing the (x, y) coordinates and the value of each cell. If the file type is SURFER files, the origin of the coordinate system for saving the file is set at the lower-left corner of the model grid. If the file type is SURFER files (real-world), the coordinates system as defined in the Environment Options dialog box (Fig. 2.105) is used.

2.7.7 Water Budget

There are situations in which it is useful to calculate flow terms for various subregions of the model. To facilitate such calculations, MODFLOW saves the computed flow terms for individual cells in the file BUDGET.DAT. These individual cell flows are referred to as cell-by-cell flow terms, and are of four types: (1) cell-by-cell stress flows, or flows into or from an individual cell due to one of the external stresses (excitations) represented in the model, e.g., pumping well or recharge; (2) cell-by-cell storage terms, which give the rate of accumulation or depletion of storage in an individual cell; (3) cell-by-cell constant-head flow terms, which give the net flow to or from individual constant-head cells; and (4) internal cell-by-cell flows, which are the flows across individual cell faces. In the file BUDGET.DAT, the flow between the cells [K, I, J] and [K, I, J+1] is denoted by FLOW RIGHT FACE, the flow between the cells [K, I, J] and [K, I+1, J] is denoted by FLOW FRONT FACE, and the flow between the cells [K, I, J] and [K+1, I, J] is FLOW LOWER FACE.

Follow the steps below to compute water budgets for the entire model, user-specified subregions, and in- and outflows between adjacent subregions.

► To calculate water budget

1. Select *Tools* | *Water Budget* to display the Water Budget dialog box (Fig. 2.94).
2. Change the settings in the Time group as needed. **PM** calculates the water budget for the given stress period and time step.
3. Click the *Subregions* button to use the Data Editor to define subregions for which a water budget is to be calculated.
   A subregion is indicated by a subregion number ranging from 0 to 50. A subregion number must be assigned to each model cell. The number 0 indicates that a cell is not associated with any subregion.
4. Once the desired subregions are defined in the Data Editor, select *File* | *Leave Editor* and save the changes.
5. Click *OK* in the Water Budget dialog box to perform the water budget calculation.

PM calculates and saves the flows in the file WATERBDG.DAT as shown in Table 2.10. The unit of the flows is $[L^3T^{-1}]$. Flows are calculated for each subregion in each layer and each time step. Flows are considered IN, if they are entering a subregion. Flows between subregions are given in a Flow Matrix. The term *HORIZ. EXCHANGE* gives the flow rate horizontally across the boundary of a subregion. The term *EXCHANGE (UPPER)* gives the flow rate coming from (IN) or going to (OUT) to the upper adjacent layer. The term *EXCHANGE (LOWER)* gives the flow

rate coming from (IN) or going to (OUT) to the lower adjacent layer. For example, consider EXCHANGE (LOWER) of REGION=1 and LAYER=1, the flow rate from the first layer to the second layer is 2.6107365E-03 m^3/s. The percent discrepancy is calculated by

$$\frac{100 \cdot (IN - OUT)}{(IN + OUT)/2} \tag{2.71}$$

2.8 The Value Menu

2.8.1 Matrix

Use the Browse Matrix dialog box (Fig. 2.95) to examine cell values. The spreadsheet displays a series of columns and rows, which corresponds to the columns and rows of the finite-difference grid. The cell data are shown in the spreadsheet. If the user is editing a particular package, in which a cell has more than one value (for example, the River package requires three values for each cell), the parameter type can be selected from the Parameter drop-down box. The Column Width drop-down box is used to change the appearance width of the columns of the spread-sheet. The cell data may be edited within the Browse Matrix dialog box. The user may also assign a value to a group of cells by using the mouse to mark the cells and then enter the desired value. The user may save the cell data by clicking the Save button and specifying the file name and the file type in a Save Matrix As dialog box. There are four file types, ASCII Matrix (Wrap form), ASCII Matrix, SURFER files and SURFER files (real-world). An ASCII Matrix file may be loaded into the spreadsheet at a later time. The format of the ASCII matrix file is described in Section 6.2.1. A SURFER file has three columns containing the (x, y) coordinates and the value of each cell. If the file type is SURFER files, the origin of the coordinate system for saving the file is set at the lower-left corner of the model grid. If the file type is SURFER files (real-world), the coordinate system defined in the the Environment Options dialog box (see Section 2.9.2) will be saved.

► To import an ASCII Matrix or a SURFER GRD file

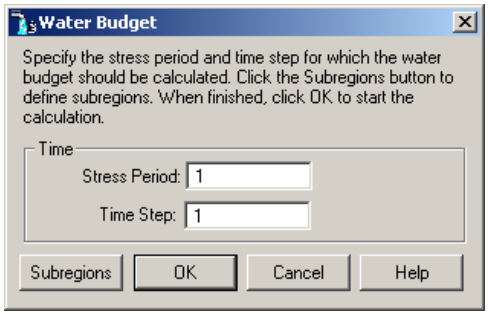

Water Budget
Specify the stress period and time step for which the water budget should be calculated. Click the Subregions button to define subregions. When finished, click OK to start the calculation.
Time
Stress Period: 1
Time Step: 1
Subregions
OK
Cancel
Help

Fig. 2.94. The Water Budget dialog box

Table 2.10 Output from the Water Budget Calculator

```
============================================================
 WATER BUDGET OF SUBREGIONS WITHIN EACH INDIVIDUAL LAYER
============================================================
 REGION   1  IN LAYER   1
------------------------------------------------
       FLOW TERM            IN            OUT         IN-OUT
   CONSTANT HEAD  1.8595711E-04  2.4354266E-04 -5.7585552E-05
               .             .             .             .
EXCHANGE (LOWER)  0.0000000E+00  2.6107365E-03 -2.6107365E-03
        RECHARGE  2.6880163E-03  0.0000000E+00  2.6880163E-03
               .             .             .             .
               .             .             .             .
SUM OF THE LAYER  2.8739735E-03  2.8542792E-03  1.9694213E-05
 DISCREPANCY [%]  0.69
               .             .             .             .
 REGION   2  IN LAYER   2
               .             .             .             .
============================================================
WATER BUDGET OF THE WHOLE MODEL DOMAIN:
============================================================
   CONSTANT HEAD  2.2167889E-03  3.7117251E-03 -1.4949362E-03
           WELLS  0.0000000E+00  1.2000003E-03 -1.2000003E-03
        RECHARGE  2.6880163E-03  0.0000000E+00  2.6880163E-03
               .             .             .             .
               .             .             .             .
------------------------------------------------------------
             SUM  4.9048052E-03  4.9117254E-03 -6.9201924E-06
 DISCREPANCY [%] -0.14

============================================================
FLOW RATES BETWEEN SUBREGIONS
============================================================
The value of the element (i,j) of the following flow
matrix gives the flow rate from the i-th region to
the j-th region. Where i is the column index and j is
the row index.

FLOW MATRIX:
           1           2
.............................
  1   2.6107E-03   0.000
  2    0.000      1.9323E-03
```

1. Click the Load button to display the Load Matrix dialog box (Fig. 2.96).
2. Click and select a file type (i.e., ASCII Matrix or SURFER GRD) and a file from an Open File dialog box.
3. Specify the starting position.
   As shown in Fig. 2.97, the starting position indicates the column and row at which a matrix will be loaded. Numbers of rows and columns of the loaded matrix need not to be identical to those of the finite-difference grid. This allows to replace only part of the cell data by the matrix. For example, the user can use the Field Generator to generate a matrix with heterogeneously distributed data from statistic parameters and load it into the grid as a subregion.
4. Select an option from the Options group. Before a matrix is loaded to the spreadsheet, its values will be modified according to the following options.

a) *Replace*: The cell data in the spreadsheet are replaced by those of the ASCII Matrix.
b) *Add*: The cell values of the ASCII Matrix are added to those of the spreadsheet.
c) *Subtract*: The cell data in the spreadsheet are subtracted from those of the loaded matrix.
d) *Multiply*: The cell data in the spreadsheet are multiplied by those of the loaded matrix.
e) *Divide*: The cell data in the spreadsheet are divided by those of the loaded matrix. If a cell value of the loaded matrix is equal to zero, the corresponding cell value in the spreadsheet remains unchanged.

Note. A SURFER GRD file may only be used with regularly spaced model grids since SURFER is limited to regular spaced grids. Furthermore, **PM** only accepts SURFER GRD files saved in ASCII. Consider using the Field Interpolator (see Section 2.7.2), if the model grid is irregularly spaced.

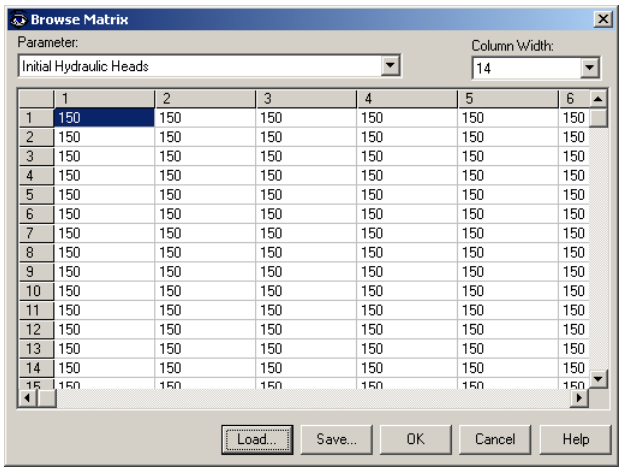


Fig. 2.95. The Browse Matrix dialog box

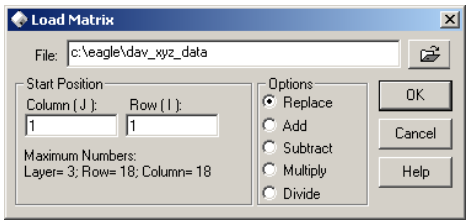


Fig. 2.96. The Load Matrix dialog box

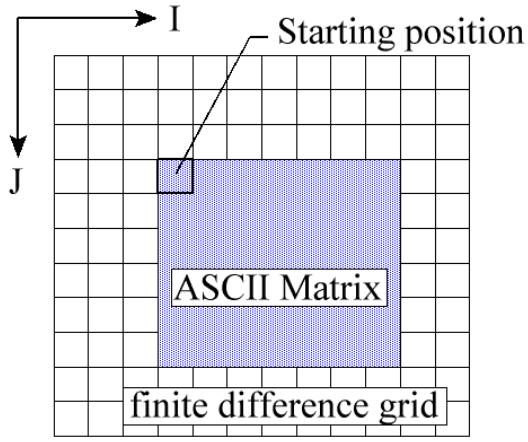


Fig. 2.97. The starting position of a loaded ASCII matrix

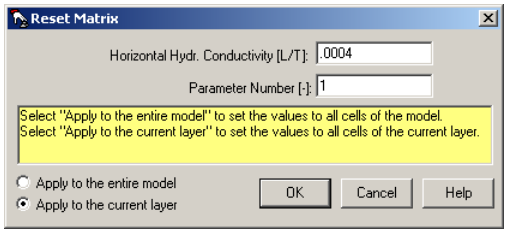

Reset Matrix
Horizontal Hydr. Conductivity [L/T]:
.0004
Parameter Number [-]:
1
Select "Apply to the entire model" to set the values to all cells of the model.
Select "Apply to the current layer" to set the values to all cells of the current layer.
Apply to the entire model
Apply to the current layer
OK
Cancel
Help

Fig. 2.98. The Reset Matrix dialog box

2.8.2 Reset Matrix

Select this menu to open the Reset Matrix dialog box (Fig. 2.98), which is used to assign uniform values to the current model layer or to the entire model. The options *Apply to the entire model* and *Apply to the current layer* are available when editing Cell Status arrays (IBOUND or ICBUND), aquifer parameters, or concentration values.

1. *Apply to the entire model*: the specified value(s) in the Reset Matrix dialog box will be applied to all cells of the entire model.
2. *Apply to the current layer* is the default option, which assigns the specified value(s) to all cells of the current layer.

2.8.3 Polygons

The Polygons menu allows the user to save or load the zones in or from a Polygon file. All polygons in the layer being edited can be deleted by selecting *Polygons | Delete All*. Using Polygon files, the user can transfer polygon information between parameters or between models with different grid configurations. The format of the polygon file is given in Section 6.2.9

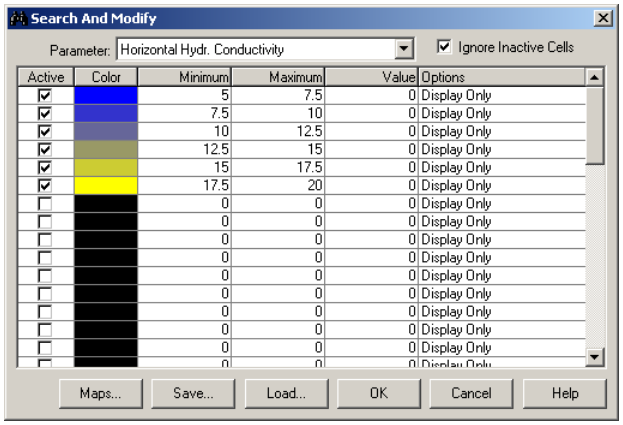


Fig. 2.99. The Search and Modify dialog box

2.8.4 Points

The Points menu appears only in the Digitizer. Refer to Section 2.7.1 for details about the Digitizer and the *Points* menu.

2.8.5 Search and Modify

Use the Search and Modify dialog box (Fig. 2.99) to modify cell data of the current layer or to create solid fill plots based on the cell data. The options of the dialog box are described below:

- *The Trace Table*: The user defines a search range and its attributes in an active row of the table. A row is active when the Active flag is checked. The search range is given by the minimum (lower limit) and the maximum (upper limit). The color in the Color column will be assigned to the finite-difference cells that have a value located within the search range.
  Regularly spaced search ranges can be assigned to each active row by clicking on one of the headers Minimum or Maximum, and then enter a minimum and a maximum value to a Search Level dialog box.
  The colors can be automatically assigned to get a gradational change from one color to another. To do this, click the header Color of the table and assign a minimum color and a maximum color to a Color Spectrum dialog box. To change the color individually, click on the colored cell (a button appears), then click on the button and select a color from a Color dialog box.
  Cell values are modified according to the user-specified value (in the Value column) and the operation option (in the Options column). The available operations are listed below:
  – *Display Only*: No operation takes place.
  – *Replace*: The cell values are replaced by the user-specified value.
  – *Add*: The user-specified value is added to the cell values.

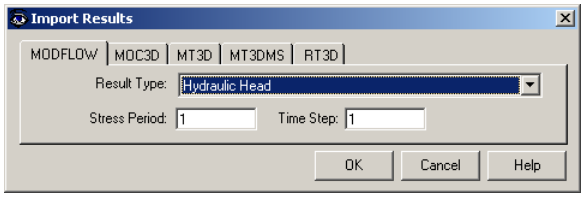


Fig. 2.100. The Import Results dialog box

  - *Multiply*: The cell values are multiplied by the user-specified value.
- *Parameter drop-down box*: For particular packages, in which a cell has more than one value (e.g., the River package of MODFLOW), this drop-down box contains the available parameter type(s). Choose the parameter type for which the Search and Modify operation will apply.
- *Ignore Inactive Cells*: If this box is checked, the Search and Modify operation will only be applied to active cells.
- *Maps*: The user may display background maps (DXF or Line Map) by using the Maps Options dialog box. See Section 2.9.1 for details.
- *Save* and *Load*: The entries in the Trace Table can be saved or loaded in trace files. The format of the trace file is given in Section 6.2.8.

2.8.6 Import Results

To import the model results select this menu item to open the Import Results dialog box (Fig. 2.100). The dialog box contains several tabs; each corresponds to a simulation model. Use these tabs to select the desired result type, simulation time, and click the OK button to import. Depends on the selected model, simulation time is expressed in terms of stress period, time step or elapsed time.

2.8.7 Import Package

When editing flow packages of MODFLOW, the user may select this menu item to import existing input files saved in the MODFLOW-88/96 format. Refer to McDonald and others [85] or Harbaugh and others [54] for input file format. The following packages are supported:

- Drain Package
- Evapotranspiration Package
- General-Head Boundary Package
- Horizontal-Flow Barrier Package
- Interbed-Storage Package
- Recharge Package
- Reservoir Package
- River Package
- Streamflow-Routing Package

- Time-Variant Specified Head Package
- Well Package

2.9 The Options Menu

There are five menu items in the Options menu - Maps, Environment, Display Cell Information, Display Mode, and Input Method. The menu item Display Cell Information opens a Cell Information dialog box (Fig. 2.8), which displays the user-specified data of the cell pointed by the grid cursor. The menu items Display Mode and Input Method are described in Section 2.2. The use of the menu items Maps and Environment is described below.

2.9.1 Map

The Maps Options dialog box (Fig. 2.101) allows the user to display up to 5 DXF-maps, 3 Line maps, and one geo-referenced raster (bitmap) graphics. The options in this dialog box are grouped under two tabs described below.

The Vector Graphics Tab

The Vector Graphics Tab is used to import DXF- or Line-maps. A DXF file contains detailed data describing numerous CAD entities. An entity is a line or symbol placed on a drawing by the CAD system. **PM** supports the following entities: LINE, POLYLINE, POINT, ARC, SOLID, CIRCLE, and TEXT. The other entities are ignored. There is no size limit to the number of the acceptable entities.

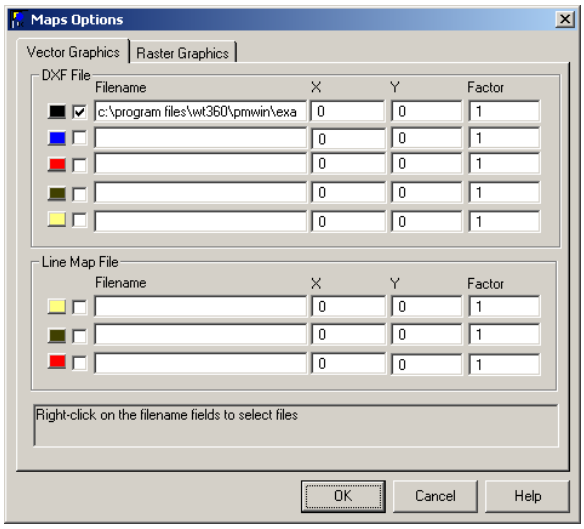


Fig. 2.101. The Map Options dialog box

A Line-Map consists of a series of polylines. Each polyline is defined by a header line and a series of coordinate pairs. The header line only contains the number of the coordinate pairs. Refer to Section 6.2.4 for the format of the Line Map files.

► To import a DXF-map or a Line map

1. Select the Vector Graphics tab.
2. Right Click on any of the DXF File or Line Map File fields and then select a file from a Map Files dialog box.
3. If necessary, use a scale factor to enlarge or reduce the appearance size of the map. Then use the values in X and Y to shift the scaled map to the desired position. For details, see the section Scaling a vector graphic below.
4. Click the colored button in the front of the edit field and select a color for the DXF-map from a Color dialog box. The color will be assigned to a DXF-graphics entity, if the entity's color is not defined in the DXF file. A line map will always use the selected color.
5. Check the box at the front of the edit field. The map will be displayed only when the box is checked.

► Scaling a vector graphic

X and Y should be 0 and Scale should be 1, if a DXF file is generated by **PM**. Since different length units are often used by various drawing or CAD software packages, DXF files created by those packages may not be correctly imported into **PM** without modifying the scale factor and the X, Y values. If these values are incorrect, a DXF-map will be displayed too small, too large or outside the Viewing Window. If this happens, use the Environment options dialog box to define a very large Viewing Window ensuring that the map can be displayed within the window. Then, check the units on the imported map by moving the mouse around the map and looking at the X and Y coordinates displayed in the status bar. Choose two points that are a known distance apart and check their distance with the status bar. If the distance is incorrect, compute a scale factor and import the map again. Once the correct scale factor is found, the user may shift the **scaled** DXF-map to the desired position by using X and Y. Fig. 2.102 uses a triangle as an example to demonstrate the use of X, Y and the scale factor.

The Raster Graphics Tab

Using the Raster Graphics tab, raster graphics saved in Windows Bitmap (*.bmp) or JPEG (*.jpg) format can be imported and geo-referenced.

► To import a raster graphics map

1. Click the Raster Graphics tab.

2. Click the open file button and select a file from a Raster Graphics dialog box.
   The map is displayed in the Maps Options dialog box (Fig. 2.103). Using the following methods to increase or decrease the magnification level of the display.
   - To move a part of the image to the center of the display, simply click the desired position.
   - To zoom in, hold down the Shift key and click the image.
   - To zoom out, hold down the Ctrl key and click the image.
   - To display entire map, hold down the Alt key and click the image.
3. Follow the steps below to set geo-reference points
   a) Click the Set button from the Point 1 or Point 2 group. The mouse pointer turns into a crosshairs.
   b) Place the crosshairs at a point with known (x, y) real-world coordinates and press the left mouse button.
   c) Enter the (x, y) coordinates into the corresponding edit fields of the group Point 1 or Point 2.
   d) Repeat the previous steps to set the other reference point. Note that the geo-reference points must not lie on a vertical or horizontal line, e.g., the x- and y-coordinates of the points must not be the same.

2.9.2 Environment

The Environment Options dialog box (Fig. 2.104) allows the user to configure the coordinate system and modify appearance of the model grid. Available settings are grouped under three tabs - Appearance, Coordinate System and Contours - which are described below. The checkbox ”Display zones in the cell-by-cell mode” is used to force **PM** to display the user-specified polygons when using the cell-by-cell input method.

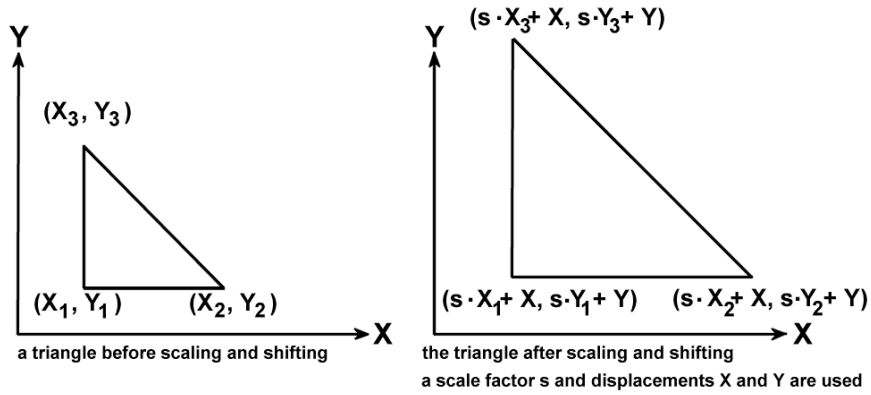


Fig. 2.102. Scaling a vector graphic

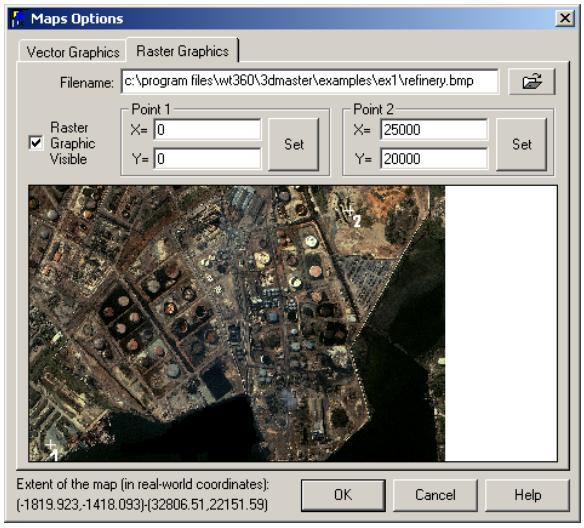


Fig. 2.103. Importing and Geo-referencing a raster map

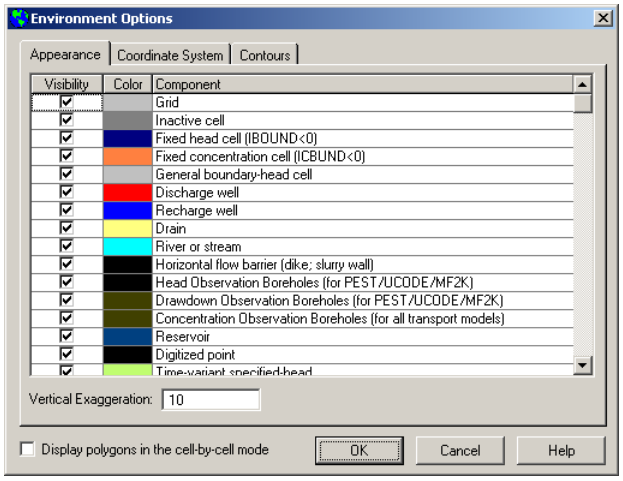


Fig. 2.104. The Appearance tab of the Environment Options dialog box

The Appearance Tab

The Appearance Tab (Fig. 2.104) allows the user to change the visibility and appearance color of each simulated component. A simulated component is visible if the corresponding Visibility box is checked. To select a new color, click on the colored cell (a button appears), then click on the button and select a color from a Color dialog box. The Vertical Exaggeration edit field controls the vertical exaggeration factor seen in the Row or Column view.

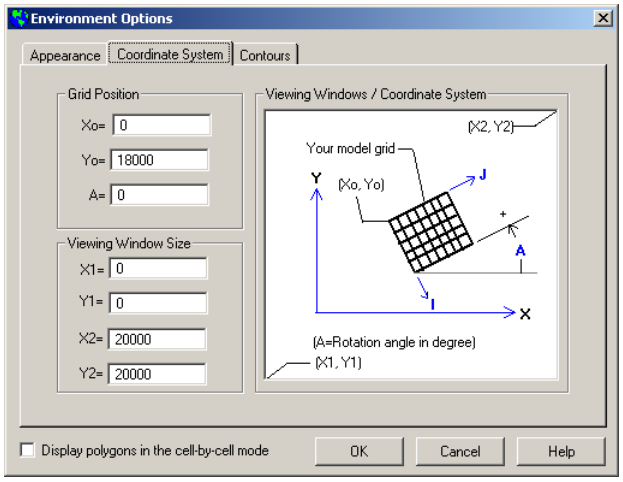


Fig. 2.105. The Coordinate System tab of the Environment Options dialog box

The Coordinate System Tab

The Coordinate System Tab is used to define the extent and location of the the Viewing Window, and to define location and orientation of the model grid.

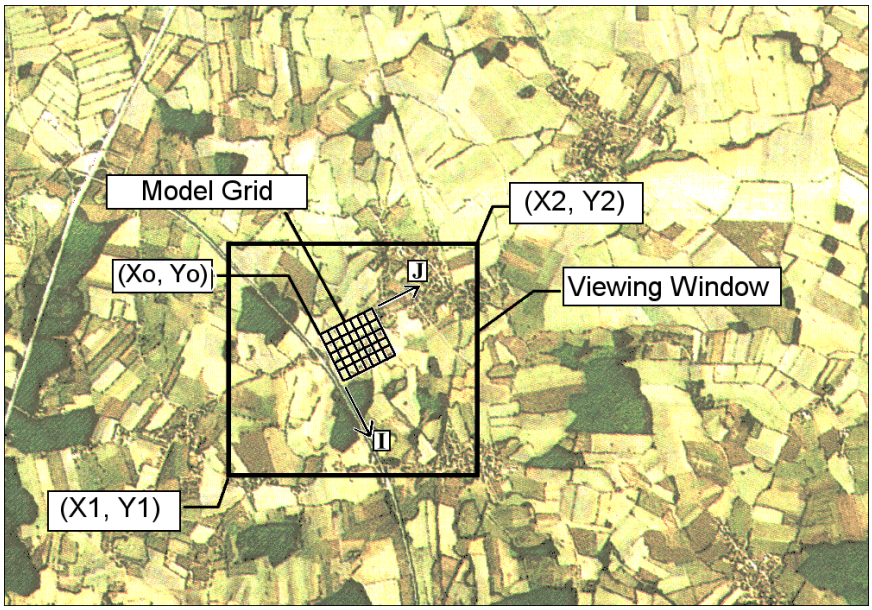


Fig. 2.106. Defining the coordinate system and orientation of the model grid

As illustrated in Fig. 2.105, the Viewing Window is a ”window” to the real-world, your model grid is placed within the Viewing Window. The extent and location of the Viewing Window are defined by specifying the (real-world) coordinates of its lower-left and upper-right corners; i.e., by the coordinates (X1, Y1) and (X2, Y2) as shown in Fig. 2.105 and Fig. 2.106. The location and orientation of the model grid are defined by the coordinates (Xo, Yo) of its left-upper corner and a rotation angle. The rotation angle is expressed in degrees and is measured counterclockwise from the positive x-direction.

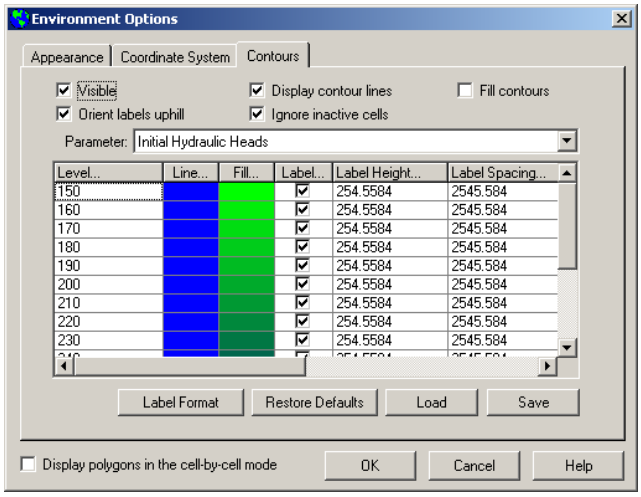


Fig. 2.107. The Contours tab of the Environment Options dialog box

The Contours Tab

The Data Editor displays contours based on the cell data. The Contours tab (Fig. 2.107) controls the display of the contour levels, labels and colors. The options of this tab are listed below.

- *Visible*: Contours are visible if this box is checked.
- *Display contour lines*: Contour lines (and labels) are displayed if this box is checked.
- *Fill contours*: Checking this box causes the space between contour lines to be filled with the color defined in the contour level table.
- *Orient label uphill*: If this box is checked, the contour labels are displayed so that they are always oriented uphill (i.e., oriented towards places with higher cell values).
- *Ignore inactive cells*: If this box is checked, the data of inactive cells will not be used for creating contours.
- *Parameter*: When editing a particular package, in which a cell has more than one value (for example, the River package requires three values for each cell), the user can select the parameter type from this drop down box. **PM** uses the data associated with the selected parameter type to create contours.
- *Contour level table*: The user may click on each cell of the table and modify the values, or click on the column header of the table to change the values for all cells of that column.
  - *Level*: To produce contours on regular intervals, click the header of this column. A Contour Levels dialog box allows the user to specify the contour range and interval. By default, this dialog box displays the lowest and high-

est values found in the current layer. After clicking OK, the contour levels in the table are updated to reflect the changes.

- *Line and Fill*: Define the color of a contour line and the fill color between two contour lines. Click on the headers Line or Fill to display the Color Spectrum dialog box (Fig. 2.108), which can be used to assign a gradational change of contour colors from the lowest contour level to the highest contour level. To change the colors correspond to the lowest or highest contour levels, simply click on one of the colored buttons and select a color from a Color dialog box. After clicking OK, the contour colors levels in the table are updated to reflect the changes.
- *Label*: Defines whether a contour should be labeled. The user may click on an individual box of the Label column to turn label on ☑ or off ☐. Click on the header to display the Contour Labels dialog box (Fig. 2.109), which can be used to define the display frequency of contour labels. *First labeled contour line* defines the first contour line to be labeled. Labeled line frequency specifies how often the contour lines are labeled. After clicking OK, the flags in the table are
- *Label height*: Specifies the appearance height of the label text. It uses the same length unit as the model.
- *Label spacing*: Specifies the distance between two contour labels. It uses the same length unit as the model.

- *Label Format*: The Label Format dialog box (Fig. 2.110) allows the user to specify the format for the labels. The elements of this dialog box are described below.
  - *Fixed*: This option displays numbers at least one digit to the left and N digits to the right of the decimal separator, where N is the value specified in Decimal digits.

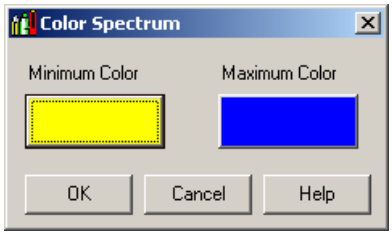


Fig. 2.108. The Color Spectrum dialog box

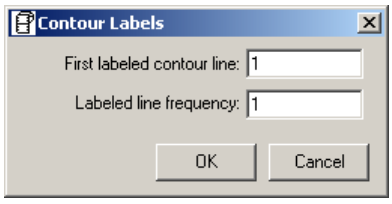


Fig. 2.109. The Contour Labels dialog box

  - *Exponential*: This option displays numbers in scientific format and E is inserted between the number and its exponent.
  - *Decimal digits*: The value of Decimal digits determines the number of digits to the right of the decimal separator. For example, if Decimal digits = 2, the value 1241.2 will be displayed as 1241.20 for the fixed option or 1.24E+03 for the exponential option.
  - *Prefix* is a text string that appears before each label.
  - *Suffix* is a text string that appears after each label.
- *Restore Defaults*: Clicking on this button, **PM** sets the number of contour lines to 11 and uses the maximum and minimum values found in the current layer as the minimum and maximum contour levels. The label height and spacing will also be set to their default values.
- *Load* and *Save*: The contents of the contour level table can be loaded from or saved in separate Contour files. Refer to Section 6.2.2 for the format.

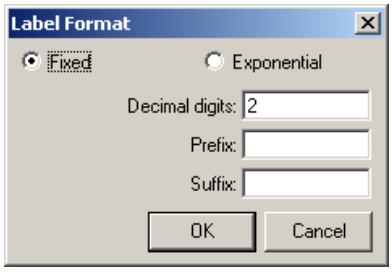


Fig. 2.110. The Label Format dialog box

3

The Advective Transport Model PMPATH

PMPATH is an advective transport model running independently from **PM**. PMPATH retrieves the groundwater models and simulation result from **PM** and MODFLOW. A semi-analytical particle-tracking scheme (Pollock [93][94]) is used to calculate the groundwater paths and travel times. Through the interactive graphical modeling environment of PMPATH, the user can place particles and perform particle tracking with just a few mouse clicks. While most available particle tracking models need post-processors for visualization of computed paths and times data, PMPATH calculates and animates the pathlines simultaneously (Fig. 3.1). Moreover, PMPATH provides various on-screen graphical options including head contours, drawdown contours and velocity vectors for any selected model layer and time step.

Both forward and backward particle tracking are allowed for steady state and transient flow simulations. For transient flow simulations, particles can start from the beginning of any time step. During the simulation, the particle-tracking algorithm will check the current time of every particle. If a particle reaches the end (forward tracking) or the beginning (backward tracking) of a time step, PMPATH forces the particle to wait, until the flow field of the next time step has been read. The particle tracking simulation proceeds until all particles have left the model via sinks or until the user-specified time limit is reached.

The time length of a single particle tracking step and the maximum number of tracking steps can be specified. Each particle can have its own color and retardation factor. With these features, PMPATH can be used to simulate advective transport in groundwater, to delineate contaminant capture zones, injection zones and wellhead protection areas or to find the point of origin of water in specified zones. PMPATH creates several output files including hydraulic heads distribution, velocity field, the x,y,z coordinates and travel times of particles. Furthermore, the coordinates along the path of each particle can be saved and used by 3D Master [23] for advanced 3D Visualization.

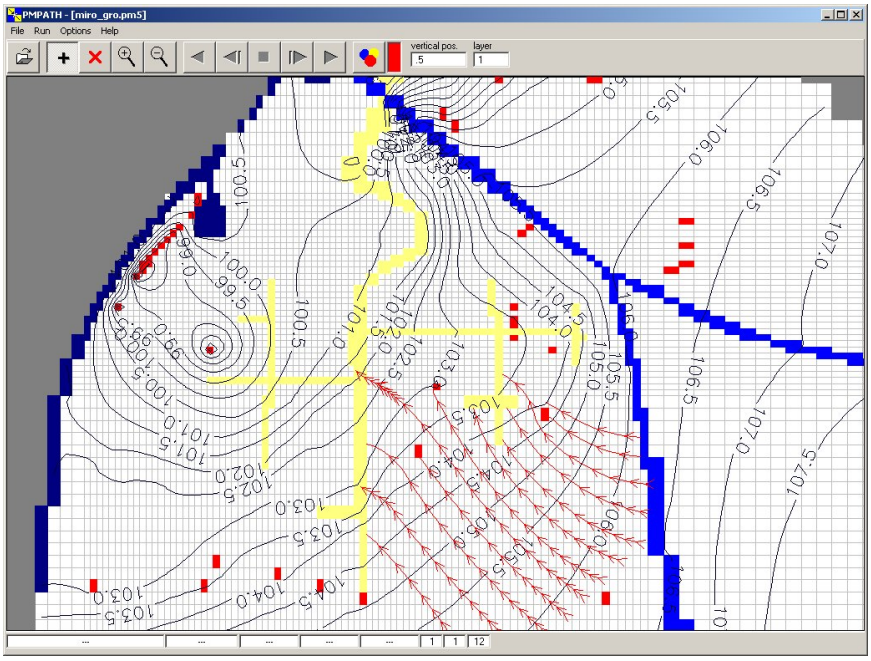


Fig. 3.1. PMPATH in action

3.1 The Semi-analytical Particle Tracking Method

Assume that the density of groundwater is constant. Consider an infinitesimal volume of a porous medium as shown in Fig. 3.2a and the law of conservation of mass. The three dimensional form of the partial differential equation for transient groundwater flow in saturated porous media at constant density can be expressed as

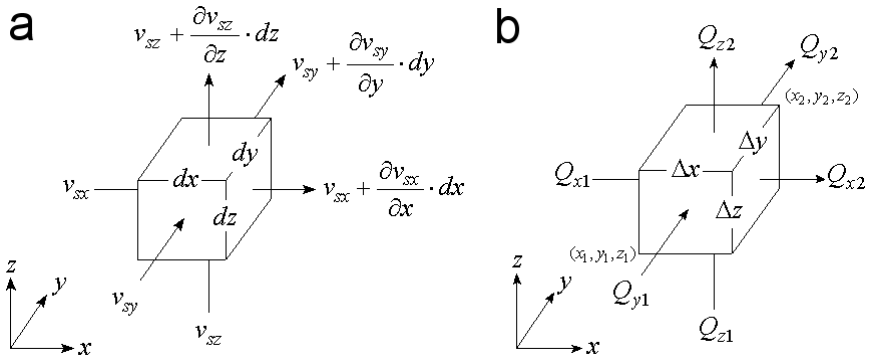


Fig. 3.2. (a) Flow through an infinitesimal volume of a porous medium and (b) the finite-difference approach

$$\frac{\partial v_{sx}}{\partial x} + \frac{\partial v_{sy}}{\partial y} + \frac{\partial v_{sz}}{\partial z} - w = S_s \frac{\partial h}{\partial t} \tag{3.1}$$

where

- v_{sx}, v_{sy}, and v_{sz} $[LT^{-1}]$ are values of the specific discharge (or Darcy velocity) through the unit volume along the x, y, and z coordinate axes;
- w $[T^{-1}]$ is a volumetric flux per unit volume and represents internal sources and/or sinks of water;
- S_s $[L^{-1}]$ is the specific storage coefficient of saturated porous media;
- h $[L]$ is the hydraulic head; and
- t $[L]$ is time.

For a three-dimensional finite-difference cell as shown in Fig. 3.2b, the finite-difference form of equation 3.1 can be written as

$$\frac{(Q_{x2} - Q_{x1})}{(\Delta y \cdot \Delta z) \cdot \Delta x} + \frac{(Q_{y2} - Q_{y1})}{(\Delta x \cdot \Delta z) \cdot \Delta y} + \frac{(Q_{z2} - Q_{z1})}{(\Delta x \cdot \Delta y) \cdot \Delta z} = \frac{W}{\Delta x \cdot \Delta y \cdot \Delta z} + S_s \frac{\Delta h}{\Delta t} \tag{3.2}$$

where

- Q_{x1}, Q_{x2}, Q_{y1}, Q_{y2}, Q_{z1}, and Q_{z2} $[L^3T^{-1}]$ are are volume flow rates across the six cell faces.
- Δx, Δy, and Δz $[L]$ are the dimensions of the cell in the respective coordinate directions;
- W $[L^3T^{-1}]$ is flow to internal sources or sinks within the cell; and
- Δh $[L]$ is the change in hydraulic head over a time interval of length Δt $[T]$.

Equation 3.2 is the volume balance equation for a finite-difference cell. The left hand side of equation 3.2 represents the net rate of outflow per unit volume of the porous medium, and the right hand side is the rate production per unit volume due to internal sources/sinks and storage. Substitution of Darcy's law for each flow term in equation 3.2 , i.e., $Q = \Delta h \cdot K \cdot A/\Delta x$, yields an equation expressed in terms of (unknown) heads at the center of the cell itself and adjacent cells. An equation of this form is written for every cell in the mesh in which head is free to vary with time. Once the system of equations is solved and the heads are obtained, the volume flow rates across the cell faces can be computed from Darcy's law. The average pore velocity components across each cell face are

$$\begin{aligned} v_{x1} &= Q_{x1}/(n_e \cdot \Delta y \cdot \Delta z) \\ v_{x2} &= Q_{x2}/(n_e \cdot \Delta y \cdot \Delta z) \\ v_{y1} &= Q_{y1}/(n_e \cdot \Delta x \cdot \Delta z) \\ v_{y2} &= Q_{y2}/(n_e \cdot \Delta x \cdot \Delta z) \\ v_{z1} &= Q_{z1}/(n_e \cdot \Delta x \cdot \Delta y) \\ v_{z2} &= Q_{z2}/(n_e \cdot \Delta x \cdot \Delta y) \end{aligned} \tag{3.3}$$

where

- n_e $[-]$ is the effective porosity, and
- v_{x1}, v_{x2}, v_{y1}, v_{y2}, v_{z1}, and v_{z2} $[LT^{-1}]$ are the average pore velocity components across each cell face.

Pollock's semi-analytical particle tracking scheme is based on the assumption that each velocity component varies linearly within a model cell in its own coordinate direction. The semi-analytical particle-tracking algorithm uses simple linear interpolation to compute the principal velocity components at any points within a cell. Given the starting location (x, y, z) of the particle and the starting time t_1 the velocity components are expressed in the form

$$\begin{aligned} v_x(t_1) &= A_x(x - x_1) + v_{x1} \\ v_y(t_1) &= A_y(y - y_1) + v_{y1} \\ v_z(t_1) &= A_z(z - z_1) + v_{z1} \end{aligned} \tag{3.4}$$

where x_1, y_1, and z_1 are defined in Fig. 3.2b. A_x, A_y, and A_z $[T^{-1}]$ are the components of the velocity gradient within the cell,

$$\begin{aligned} A_x &= (v_{x2} - v_{x1})/\Delta x \\ A_y &= (v_{y2} - v_{y1})/\Delta y \\ A_z &= (v_{z2} - v_{z1})/\Delta z \end{aligned} \tag{3.5}$$

Using a direct integration method described in Pollock [93] and considering the movement of the particle within a cell, the particle location at time t_2 is

$$\begin{aligned} x(t_2) &= x_1 + \left(v_x(t_1) \cdot e^{A_x \cdot \Delta T} - v_{x1}\right)/A_x \\ y(t_2) &= y_1 + \left(v_y(t_1) \cdot e^{A_y \cdot \Delta T} - v_{y1}\right)/A_y \\ z(t_2) &= z_1 + \left(v_z(t_1) \cdot e^{A_z \cdot \Delta T} - v_{z1}\right)/A_z \end{aligned} \tag{3.6}$$

where $\Delta T = t_2 - t_1$.

For steady-state flow fields, the location of the particle at time t_2 must still be within the same cell as at time t_1. Given any particle's starting location within a cell at time t_1, Pollock's algorithm allows determining the particle's exit time t_2 and exiting point from the cell directly, without having to calculate the actual path of the particle within the cell.

The particle tracking sequence is repeated until the particle reaches a discharge point or until a user-specified time limit is reached. Backward particle tracking is implemented by multiplying all velocity terms in equation 3.3 by -1.

For transient flow fields, in addition to the condition for steady-state flow fields, t_1 and t_2 must lie within the same time step. In PMPATH, each particle may be associated with a set of attributes, i.e., the retardation factor, the starting, forward and backward travel times and positions. If a particle is traveling across the end (forward tracking) or the beginning (backward tracking) of a time step of a flow simulation, PMPATH sets t_2 to the end or beginning time of this time step and forces the particle to wait until the flow field of the next time step (forward tracking) or the previous

time step (backward tracking) is read. If the end or beginning time of a transient flow simulation is reached, the most recent flow field can be treated as steady state and the movement of particles can go on.

3.1.1 Consideration of the display of the calculated pathlines

Because of the capability of calculating a particle's exit point from a cell directly, pathlines displayed by PMPATH may sometimes intersect each other. Consider the case shown in Fig. 3.3, two particles within a two-dimensional cell start at the same time. The dashed curves represent the actual paths of these two particles. The solid lines are the pathlines displayed by PMPATH. The pathlines intersect each other, although the particles' exit points are exactly equal to that of the actual paths. This spurious effect can be prevented by using a smaller particle tracking step length such that intermediate particle positions between starting point and exit point can be calculated. See Particle Tracking (Time) Properties dialog box (Section 3.3.2) for how to change the particle tracking step length.

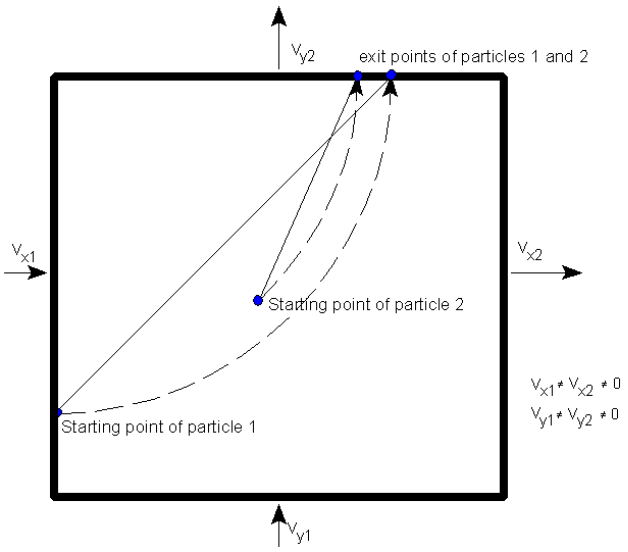


Fig. 3.3. Schematic illustration of the spurious intersection of two pathlines in a two-dimensional cell

3.1.2 Consideration of the spatial discretization and water table layers

The method described above is based on the assumption that the model domain was discretized into an orthogonal finite-difference mesh, i.e., all model cells in the same layer have the same thickness. In practice, variable layer thickness is often preferred

for approaching varying thickness of stratigraphic geohydrologic units. In order to calculate approximate groundwater paths for this kind of discretization, PMPATH uses a local vertical coordinate instead of the real-world z-coordinate. The local vertical coordinate is defined for each cell as

$$Z_L = (z - z_1)/(z_2 - z_1) \tag{3.7}$$

where z_1 and z_2 are the elevations of the bottom and top of the cell, respectively. According to this equation, the local vertical coordinate z_L is equal to 0 at the bottom of the cell and is equal to 1 at the top of the cell.

For water table layers, z_2 is set equal to the head in the cell. In MODFLOW, model layers of type 1 (unconfined) are always water table layers; model layers of type 2 or 3 (confined/unconfined) are water table layers when the hydraulic head in the cell is beneath the elevation of the cell top.

When a particle moves laterally from one cell to another, the exit point in the one and the entry point in the other cell have the identical local vertical coordinates. This causes vertical discontinuities of pathlines if bottoms and tops of cells of the neighboring cells are different. This discontinuity does not introduce error; it is merely unesthetic. It can be kept small, if the discretization is kept fine enough to have relatively small cell-to-cell variations of bottoms and tops.

3.2 PMPATH Modeling Environment

The PMPATH modeling environment (Fig. 3.4) consists of the Worksheet, the cross-section windows, the tool bar and the status bar. They are described in the following sections.

3.2.1 Viewing Window and cross-section windows

PMPATH as well as **PM** use the same spatial discretization convention as MODFLOW. An aquifer system is discretized into mesh blocks, or cells. An [K, I, J] indexing system is used to describe the locations of cells in terms of layers, rows, and columns. The K-, I-, and J-axes are oriented along the layer, row, and column directions, respectively. The origin of the cell indexing system is located at the upper, top, left cell of the model. MODFLOW numbers the layers from the top down, an increment in the K index corresponds to a decrease in elevation z.

PMPATH always displays the model grid parallel to the Viewing Window, while the user may shift and rotate a model grid by giving the rotation angle A and the coordinates (Xo, Yo) of the upper-left corner of the grid. The relation between the model grid and the real-world (x, y, z) coordinate system is illustrated in Fig. 3.4. The Viewing Window displays the plan view of the current model layer and the projection of pathlines on the horizontal plane. The cross-section windows display the projection of pathlines on the IK- and JK-planes. The Environment Options dialog

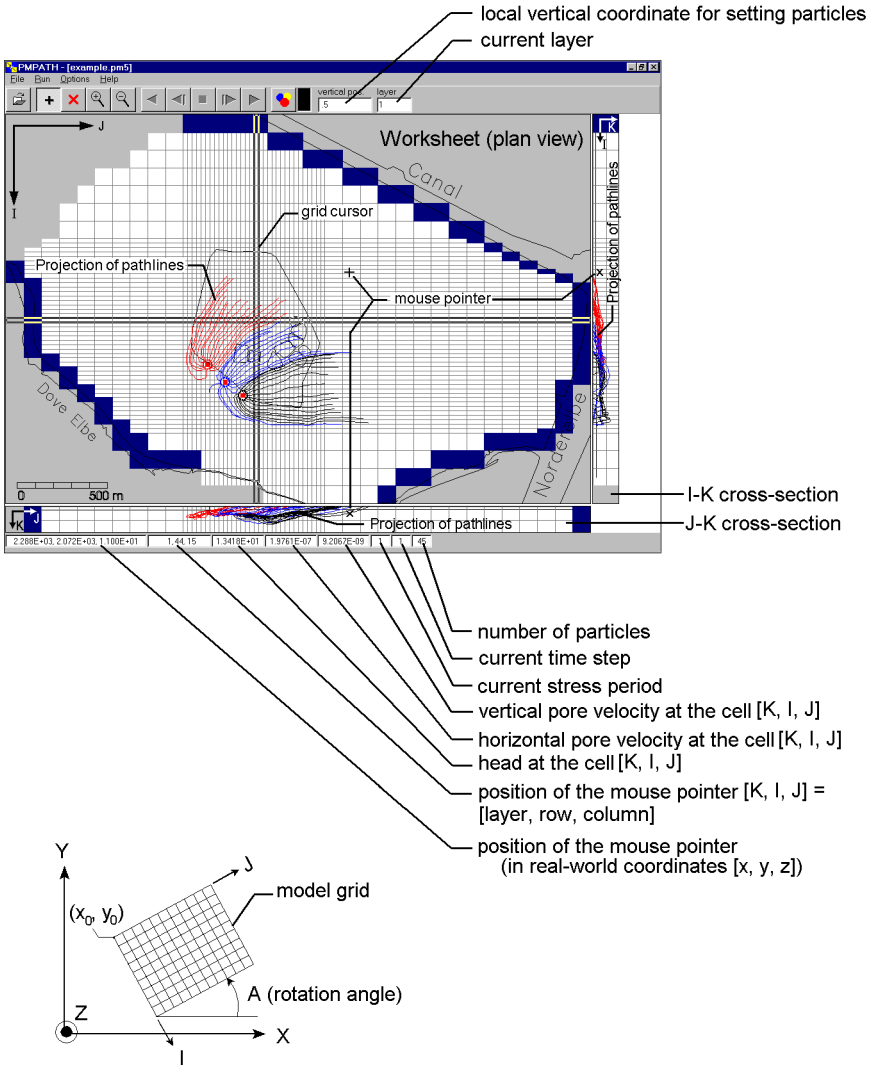


Fig. 3.4. The PMPATH modeling environment

box of PMPATH (see Section 3.3.1) allows the user to change the appearance of these windows.

The projection of pathlines on the cross-sections is useful when running PMPATH with a three-dimensional (multi-layer) flow field. The user should always keep in mind that only the projections of pathlines are displayed. The projection of a pathline may be intersected by another or even itself, particularly if a three-dimensional flow field or a transient flow field is used.

3.2.2 Status bar

The Status bar displays the following messages:

1. Current position of the mouse pointer (in both [x, y, z] coordinates and [K, I, J] indices),
2. Hydraulic head at the cell [K, I, J],
3. Average horizontal pore velocity at the center of the cell [K, I, J],
4. Average vertical pore velocity at the center of the cell [K, I, J],
5. Current stress period of the flow simulation,
6. Current time step of the flow simulation, and
7. Number of particles.

See Particle Tracking (Time) Properties dialog box (Section 3.3.2) for how to change the current stress period and time step. The hydraulic heads at the current stress period and time step are calculated by MODFLOW. The x and y components of the average horizontal pore velocity at the center of a cell is obtained by averaging the velocities v_{x1}, v_{x2} and v_{y1}, v_{y2} respectively (Equation 3.3). The average vertical pore velocity at the center of a cell is the average of the velocities v_{z1}, v_{z2} (Equation 3.3). The vertical velocity is defined as positive when it points in the K-direction.

3.2.3 Tool bar

The tool bar provides quick access to commonly used commands in the PMPATH modeling environment. You click a button on the tool bar once to carry out the action represented by that button. To change the current layer or the local vertical coordinate, click the corresponding edit field in the tool bar and type the new value then press ENTER. See equation 3.7 for the definition of the local vertical coordinate. Table 3.1 summarizes the use of the tool bar buttons, which are described in the following sections.

3.2.3.1 Open model

The Open model button opens an existing model created by **PM**. A model file for **PM** always has the extension PM5. Prior to opening a model, the flow simulation must be performed. By default, PMPATH reads the unformatted (binary) files (HEADS.DAT and BUDGET.DAT) from the same folder as the loaded model.

Note. The first time PMPATH is started from **PM**, the model currently used by **PM** will be loaded into PMPATH automatically. If model data has been modified and a flow simulation has been performed, the modified model must be re-loaded into PMPATH to ensure that it can recognize the modifications.

Table 3.1 Summary of the toolbar buttons of PMPATH

Button	Name	Action
	Open model	Opens a model created by PMWIN.
	Set Particle	Allows the user to place particles in the model domain.
	Erase particle	Activates the erase particle tool.
	Zoom in	Allows the user to drag a zoom-window over a part of the model domain..
	Zoom out	Forces PMPATH to display the entire model grid.
	Particle color	Allow the user to select a color for new particles from a color dialog box.
	Run particles backward	Execute backward particle tracking for a time length. The product of the number of particle tracking steps and the particle tracking step length defines the time length.
	Run particles backward step by step	Execute backward particle tracking for a user-specified particle tracking step length.
	Stop particle-tracking	Stop the particle tracking or stops drawing particles.
	Run particles forward step by step	Execute forward particle tracking for a user-specified particle tracking step length.
	Run particles forward	Execute forward particle tracking for a time length. The product of the number of particle tracking steps and the particle tracking step length defines the time length.

3.2.3.2 Set particle

Use the following two methods to place particles in the current layer. The current layer is shown in the tool bar (Fig. 3.4). Change it first, if particles need to be placed in another layer. Note that particles cannot be placed in inactive cells or fixed-head cells (constant head cells).

► To place a group of particles

1. Click the Set particle button .
2. Move the mouse pointer to the active model area. The mouse pointer turns into crosshairs.
3. Place the crosshairs where the user wants a corner of the ”Set Particle” window.
4. Drag the crosshairs until the window covers the sub-region over which particles will be placed, then release the mouse button.

The Add New Particles box appears (Fig. 3.5). Where NK, NI, and NJ are the number of particles in layer, row, and column directions, respectively. Particles can be placed either on cell faces or within cells, which lie in the "Set Particle" window. These numbers NK, NI, and NJ can range from 0 to 999. In the case shown in Fig. 3.5, 8 (= 2 × 2 × 2) particles will be placed within each cell, 3 (= 3 × 1) particles will be placed on each cell face, and 15 particles will be placed around each cell at a distance of 20. The particles will get the color and the retardation factor given in the Properties tab of this dialog box.

► To place a single particle

1. Click the Set particle button [+].
2. Change the local vertical coordinate and the particle color (for the definition of the local vertical coordinate, see equation 3.7).
3. Place a particle by right-clicking the desired position. This particle will have the retardation factor (see below) specified in the Properties tab of the Add New Particles dialog box. Once particles are placed, their color and retardation factor cannot be changed any more.

The retardation factor R is defined by

$$R = 1 + \frac{\rho_b}{n_e} \cdot K_d \tag{3.8}$$

where ρ_b is the bulk density of the porous medium, n_e is the effective porosity, and K_d is the distribution coefficient. A detailed description of these parameters can be found in the literature, e.g., Freeze and Cherry [46]. The retardation factor was first applied to groundwater problems by Higgins [58] and Baetsle [11]. Baetsle indicated that it may be used to determine the retardation of the center of mass of a contaminant moving from a point source while undergoing adsorption. PMPATH

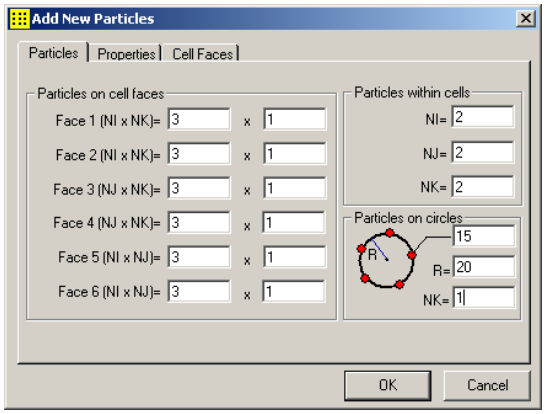


Fig. 3.5. The Add New Particles dialog box

uses the retardation factor to modify the average pore velocity of the groundwater flow. The velocity vectors in Equation 3.3 become

$$\begin{aligned} v_{x1} &= Q_{x1}/(n_e \cdot \Delta y \cdot \Delta z)/R \\ v_{x2} &= Q_{x2}/(n_e \cdot \Delta y \cdot \Delta z)/R \\ v_{y1} &= Q_{y1}/(n_e \cdot \Delta x \cdot \Delta z)/R \\ v_{y2} &= Q_{y2}/(n_e \cdot \Delta x \cdot \Delta z)/R \\ v_{z1} &= Q_{z1}/(n_e \cdot \Delta x \cdot \Delta y)/R \\ v_{z2} &= Q_{z2}/(n_e \cdot \Delta x \cdot \Delta y)/R \end{aligned} \tag{3.9}$$

3.2.3.3 Erase Particle

The user can only erase particles located in the current layer. The current layer is shown in the tool bar. Change it first, if the user needs to erase particles in another layer.

► To erase particles

1. Click the Erase particle button .
2. Move the mouse pointer to where the user wants a corner of the ”Erase” window.
3. Drag the mouse pointer until the window covers the particles to be deleted.
4. Release the mouse button.

3.2.3.4 Zoom In

By default, PMPATH displays the entire model grid. Zoom in is useful for viewing a part of the model domain in greater detail or for saving plots of a certain part of the model area (see Section 3.4.1 for how to save plots).

► To zoom in on a part of the model

1. Click the Zoom In button .
2. Move the mouse pointer to where the user wants a corner of the ”Zoom” window.
3. Drag the mouse pointer until the window covers the model area to be displayed.
4. Release the mouse button.

3.2.3.5 Zoom Out

Clicking on the Zoom Out button forces PMPATH to display the entire model grid.

3.2.3.6 Particle Color

Clicking on the Particle color button allows the user to select a color for new particles from a Color dialog box. Particles with different colors are useful for determining the capture zones of various pumping wells. In this case, particles with a certain color are placed around or on the cell-faces of each pumping well. Through backward tracking, capture zones of each pumping well can be recognized by their different colors.

3.2.3.7 Run Particles Backward

Click to execute backward particle tracking for a specified time length. The time length is the product of the number of particle tracking steps and the particle tracking step length given in the Particle Tracking (Time) Properties dialog box. See Section 3.3.2 for details.

3.2.3.8 Run Particles Backward Step by Step

Click to move particles backward a single particle-tracking step. The particle tracking step length is defined in the Particle Tracking (Time) Properties dialog box. See Section 3.3.2 for details.

3.2.3.9 Stop Particle Tracking

Click to stop particle tracking or stop redrawing particles when this button is highlighted (i.e., the rectangle on the button is colored in red).

PMPATH redraws the particles whenever the PMPATH window has been covered by other windows and becomes visible again. For example, if the user switches to to another application and then returns to PMPATH, it will redraw all particles. If too many particles are placed, it might be necessary to keep PMPATH from redrawing all of the particles all over again.

Under some circumstances, PMPATH will take a long time to calculate the coordinates of flow paths and travel times. This is especially true, if the flow velocities and the user-specified time step length of particle track-ing are very small. Click the Stop Particle Tracking button, if the particle tracking simulation appears too slow.

3.2.3.10 Run Particles Forward Step by Step

Click to move particles forward a single particle tracking step. The particle tracking step length is defined in the Particle Tracking (Time) Properties dialog box. See Section 3.3.2 for details.

3.2.3.11 Run Particles Forward

Click ▶ to execute forward particle tracking for a specified time length. The time length is the product of the number of particle tracking steps and the particle tracking step length given in the Particle Tracking (Time) Properties dialog box. See Section 3.3.2 for details.

3.3 PMPATH Options Menu

3.3.1 Environment

The Environment Options dialog box (Fig. 3.6) allows modifying the appearance of the model. The available settings are grouped under 4 tabs; namely Appearance, Cross Sections, Velocity vectors and Contours. These tabs are described below.

The Appearance Tab

The Appearance Tab (Fig. 3.6) allows changing the visibility and appearance color of each simulated component. A simulated component is visible if the corresponding Visibility box is checked. To select a new color, click on the colored cell (a ▼ button appears), then click on the ▼ button and select a color from a Color dialog box.

The Cross Sections Tab

The options of the Cross Sections tab (Fig. 3.7) is given below.

- *Visible*: Check this box to display the cross section windows. If the model thickness or the exaggeration value (see below) is too small such that the appearance

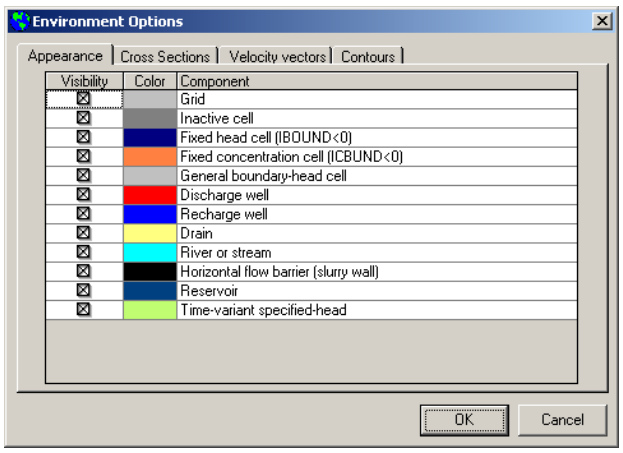


Fig. 3.6. The Environment Options dialog box of PMPATH

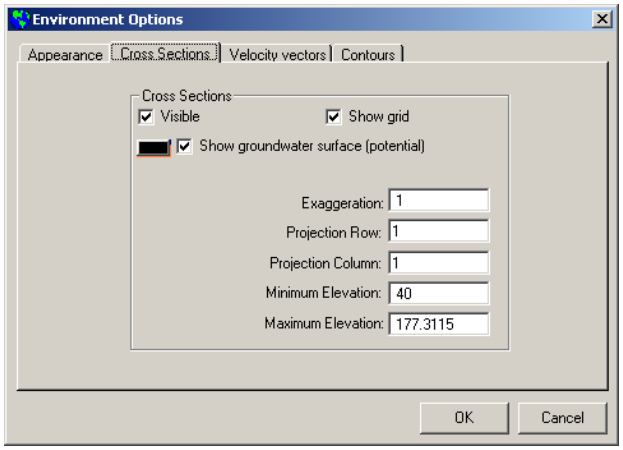


Fig. 3.7. The Cross Sections tab of the Environment Options dialog box of PMPATH

thickness on the screen is smaller than 1 pixel, PMPATH will clear this box and turn off the display of the cross sections. In this case, the Visible check box will be cleared automatically.

- *Show grid*: Check this box to display the model grid.
- *Show Groundwater surface (Potential)*: Check this box to display the groundwater surface (or the hydraulic heads of the highest active cells) on the cross sections.
- *Exaggeration (scaling factor for the height)*: Use this value to change the appearance height of the cross sections. A larger exaggeration value lets PMPATH draw the projection of the pathlines on the cross section windows in greater details. The exaggeration value can range from 0.01 to 1000.
- *Projection Row* and *Projection Column*: PMPATH uses the grid cursor (Fig. 3.4) to define the column and row for which the cross sectional plots should be made. The grid cursor can be moved by holding down the Ctrl-key and click the left mouse button on the desired position. Alternatively, type the row and column in the Projection Row and Projection Column edit boxes.
- *Minimum Elevation* and *Maximum Elevation*: The visible part on the cross sectional plots is defined by Minimum Elevation and Maximum Elevation. By default, the maximum elevation is set to the highest elevation of the model grid (or the largest hydraulic head). The minimum elevation is set to the lowest elevation of the model grid (or the smallest hydraulic head).

The Velocity Vectors Tab

Velocity vectors describe the direction of water movement at any instant of a given time step of the simulation (see Section 3.3.2 for the definition of time step). Checking the Visible check box, the projection of velocity vectors of each active model cell will be displayed on the Viewing Window and cross section windows. Click the color

button next to the Visible check box to change the appearance color of the velocity vectors. The appearance size of the largest velocity vector is defined by the Vector size (in pixels), which defaults to 25 and can be ranged from 1 to 32767.

The Contours Tab

PMPATH displays contours based on the calculated hydraulic head or drawdown values. The Contours tab (Fig. 3.8) controls the display of the contour levels, labels and colors. The options of this tab are listed below.

- *Visible*: Contours are visible if this box is checked.
- *Orient label uphill*: If this box is checked, the contours labels are displayed so that they are always oriented uphill (i.e., oriented towards places with higher cell values).
- *Head* or *Drawdown*: Use the options Head or Drawdown to decide which kind of contours should be displayed.
- *Contour level table*: The user may click on each cell of the table and modify the values, or click on the column header of the table to change the values for all cells of that column.
  - *Level*: To produce contours on regular intervals, click the header of this column. A Contour Levels dialog box allows the user to specify the contour range and interval. By default, this dialog box displays the lowest and highest values found in the current layer. After clicking OK, the contour levels in the table are updated to reflect the changes.
  - *Color*: Defines the color of a contour line. Click on the header to display the Color Spectrum dialog box (Fig. 3.9), which can be used to assign a gradational change of contour colors from the lowest contour level to the highest contour level. To change the colors correspond to the lowest or highest con-

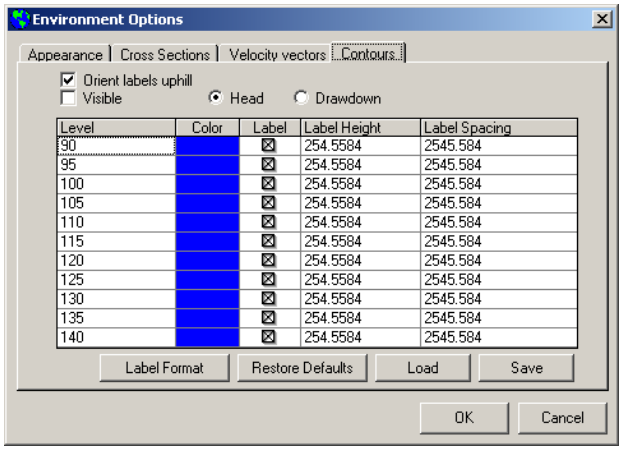


Fig. 3.8. The Contours tab of the Environment Options dialog box of PMPATH

tour levels, simply click on one of the colored buttons and select a color from a Color dialog box. After clicking OK, the contour colors levels in the table are updated to reflect the changes.
  - *Label*: Defines whether a contour should be labeled. The user may click on an individual box of the Label column to turn label on ☑ or off ☐. Click on the header to display the Contour Labels dialog box (Fig. 3.10), which can be used to define the display frequency of contour labels. *First labeled contour line* defines the first contour line to be labeled. Labeled line frequency specifies how often the contour lines are labeled. After clicking OK, the flags in the table are updated to reflect the changes.
  - *Label height*: Specifies the appearance height of the label text. It uses the same length unit as the model.
  - *Label spacing*: Specifies the distance between two contour labels. It uses the same length unit as the model.
  - *Label height* specifies the appearance height of the label text. It uses the same length unit as the model.
  - *Label spacing* specifies the distance between two contour labels. It uses the same length unit as the model.
- *Label Format*: The Label Format dialog box (Fig. 3.11) allows the user to specify the format for the labels. The options of this dialog box are described below.
  - *Fixed*: This option displays numbers at least one digit to the left and N digits to the right of the decimal separator, where N is the value specified in Decimal digits.
  - *Exponential*: This option displays numbers in scientific format and E is inserted between the number and its exponent.

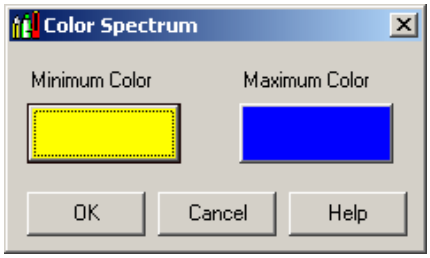


Fig. 3.9. The Color Spectrum dialog box

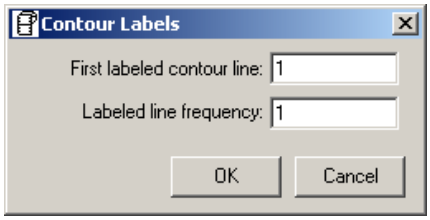


Fig. 3.10. The Contour Labels dialog box

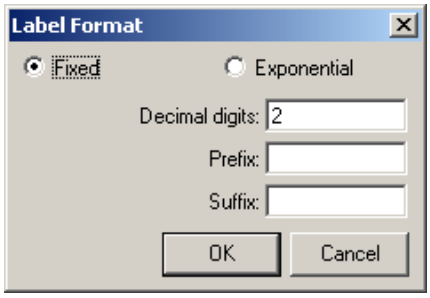


Fig. 3.11. The Label Format dialog box

  - *Decimal digits*: The value of Decimal digits determines the number of digits to the right of the decimal separator. For example, if Decimal digits = 2, the value 1241.2 will be displayed as 1241.20 for the fixed option or 1.24E+03 for the exponential option.
  - *Prefix* is a text string that appears before each label.
  - *Suffix* is a text string that appears after each label.
- *Restore Defaults*: Clicking on this button, PMPATH sets the number of contour lines to 11 and uses the maximum and minimum values found in the current layer as the minimum and maximum contour levels. The label height and spacing will also be set to their default values.
- *Load* and *Save*: The contents of the contour level table can be loaded from or saved to separate Contour files. Refer to Section 6.2.2 for the format.

3.3.2 Particle Tracking (Time)

The available settings of the Particle Tracking (Time) dialog box (Fig. 3.12) are grouped under three tabs - Simulation Mode/Time, Pathline Colors, and RCH/EVT options. These tabs are described below.

The Simulation Mode/Time Tab

The options of the Simulation Mode/Time tab (Fig. 3.12) are described below.

- *Current Time*: In MODFLOW, simulation time is divided into stress periods, which are in turn divided into time steps. The time length of each stress period and time step is defined in **PM**. In PMPATH, the user can move to any stress period and time step as long as the resulting heads and budget data are saved for that stress period/time step. The starting time of each particle is always the beginning of the time step defined in Current Time.
- *Tracking Step*: To select a time unit for Step length, click the down arrow on the Unit drop down box. The step length is the time length that particles may move when one of the buttons or is pressed. Maximum steps is the allowed number of particle tracking steps. Each time one of the buttons or is pressed,

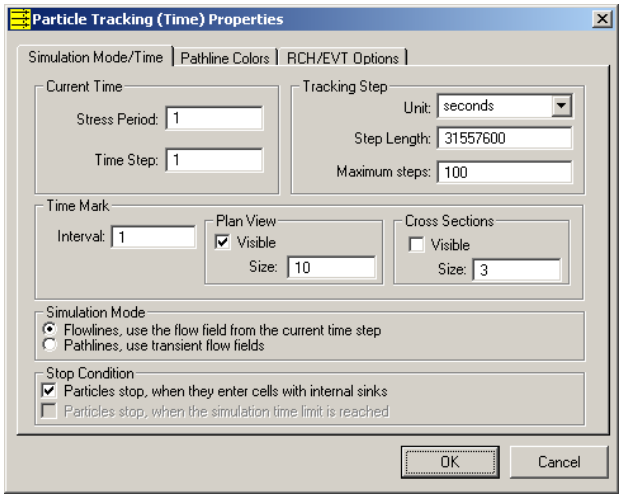


Fig. 3.12. The Particle Tracking (Time) dialog box

particles will move backward or forward for a time length defined by the product of Step length and Maximum steps.

- *Time Mark*: PMPATH places a time mark on pathlines for each n-th tracking step, where n is given in Interval. Check the corresponding Visible boxes to see time marks on the Viewing Window or the cross section windows. The appearance size of the time marks is defined by Size (in pixels). The default value of Size is 10 for the Viewing Window and 3 for the cross section windows. The sizes can be ranged from 1 to 2,147,483,647.
- *Simulation Mode*: PMPATH can be used to calculate flowlines or pathlines. Flowlines indicate the instantaneous direction of flow throughout a system (at all times of a steady state flow simulation or at a given time step of a transient flow simulation). Pathlines map the route that an individual particle of water follows through a region of flow under steady state or transient conditions. In a steady state flow system pathlines will coincide with flowlines. In this case, only the option ”Flowline, use the flow field from the current time step” is available. In the case of a transient flow simulation where groundwater flow varies from time step to time step, the flowlines and pathlines do not coincide. Use the option ”Pathlines, use transient flow fields” to calculate transient pathlines.
- *Stop Conditions*: In general, particles will stop when the allowed travel time defined in Tracking Step is reached or when the particles reach specified head cells. In addition to these conditions, two stop conditions are available:
  - *Particles stop, when they enter cells with internal sinks*: The flow model MODFLOW includes the options to simulate wells, drains, rivers, general head boundaries, streams, evapotranspiration and recharge. Except the last two options, they are treated as internal distributed sources or sinks by PMPATH. If the internal sink of a cell is sufficiently strong, flow will be into the

cell from all cell faces. In that case, every particle that enters the cell will be discharged. If the sink is weak, flow will be into the cell from some cell faces and a part of the flow will leave the cell through other faces. A particle entering such a cell may be discharged or may leave the cell again. In the finite difference approach, however, it is impossible to determine whether that particle should be discharged or pass through the cell. If this option is selected, particles will be discharged when they enter cells with internal sinks, regardless of the flow condition.

– *Particles stop, when the simulation time limit is reached*: This option is available only if the simulation mode "Pathlines, use transient flow fields" is selected. In PMPATH, the starting time of each particle is always the beginning of the time step defined in Current Time. For the forward particle-tracking scheme, the simulation time limit is the end of a transient flow simulation. For the backward particle-tracking scheme, on the other hand, the simulation time limit is the beginning of the simulation. Backward particle tracking will not work, if this stop option is checked and particles are started from the beginning of a transient flow simulation. In this case, particles will be stopped immediately after the start. Note that PMPATH cannot start backward particle tracking from the end of a transient flow simulation, rather PMPATH can only start particles from the beginning of the last simulation time step. If the simulation time limit is reached and this option is not checked, PMPATH calculates flowlines by assuming that the flow field of the first or last time step is steady state.

The Pathline Colors Tab

Normally, the color of each pathline is the same as the color of each particle. However, it is sometimes useful when the colors of pathlines are distinguished by layers instead of particles. There are two ways to change the color of each layer:

► To change the color individually

1. Click on a colored cell of the table (Fig. 3.13), a button appears in the cell.
2. Click on the button and select a color from a Color dialog box.

► To Change the color using the Color Spectrum dialog box

1. Click the header button *Color*.
   A Color Spectrum dialog box appears. Using the Color Spectrum dialog box, the color of each layer can be automatically assigned to get a gradational change from one color to another.
2. In the Color Spectrum dialog box, click the Minimum Color button to display a Color dialog box. In the Color dialog box, select a color and click OK. Repeat this procedure for the Maximum Color button.
3. In the Color Spectrum dialog box, click OK. A gradation of colors from the minimum to the maximum is assigned to each layer.

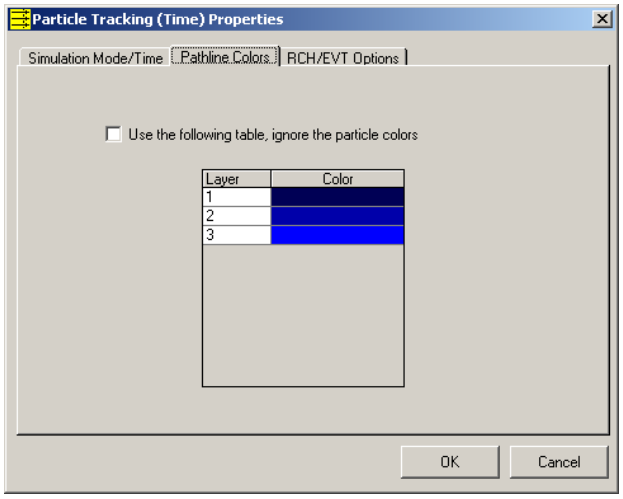


Fig. 3.13. The Pathline Colors tab of the Particle Tracking (Time) dialog box

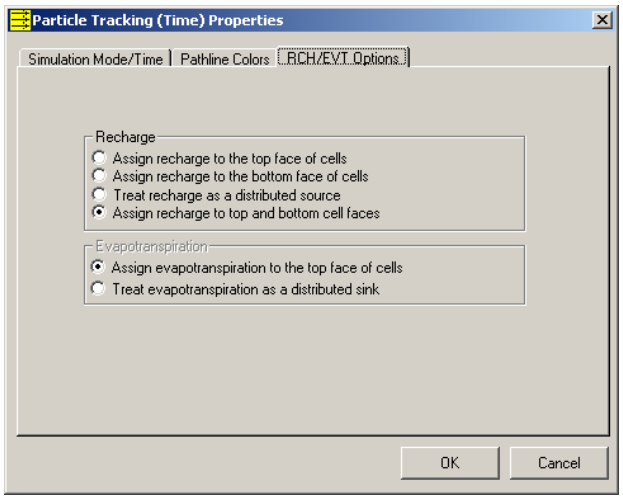

Particle Tracking (Time) Properties
Simulation Mode/Time
Pathline Colors
RCH/EVT Options
Recharge
Assign recharge to the top face of cells
Assign recharge to the bottom face of cells
Treat recharge as a distributed source
Assign recharge to top and bottom cell faces
Evapotranspiration
Assign evapotranspiration to the top face of cells
Treat evapotranspiration as a distributed sink
OK
Cancel

Fig. 3.14. The RCH/EVT Options tab of the Particle Tracking (Time) dialog box

The RCH/EVT Options Tab

The RCH/EVT Options tab (3.14) provides two options:

- *Recharge*: The option is disabled if recharge is not used. MODFLOW treats recharge as an internal distributed source of a cell and does not assign it to any of the six cell faces. The distributed source approximation is usually only appropriate for two dimensional areal flow models. The flow velocity across the top face of a cell in the top model layer is zero, if the existing recharge is not assigned to the top face. Consequently, particles cannot be tracked backwards to the top

face. In PMPATH, recharge may be treated as a distributed source, or assigned to the top face or bottom face of a cell by selecting a corresponding option from the dialog box. If the option ”Assign recharge to top and bottom cell faces” is chosen, positive recharge values will be assigned to the top face and ”negative” recharge values will be assigned to the bottom face.

- *Evapotranspiration*: The option is disabled if evapotranspiration is not used. Similar to Recharge, evapotranspiration can be assigned to top face of a cell or treated as a distributed sink.

3.3.3 Maps

The Maps Options dialog box (Fig. 3.15) allows the user to display up to 5 DXF-maps and 3 Line Maps. A DXF-file contains detailed data describing numerous CAD entities. An entity is a line or symbol placed on a drawing by the CAD system. PMPATH supports the following entities: LINE, POLYLINE, POINT, ARC, SOLID, CIRCLE, and TEXT. The other entities are ignored. There is no size limit to the number of the acceptable entities.

A Line Map consists of a series of polylines. Each polyline is defined by a header line and a series of coordinate pairs. The header line only contains the number of the coordinate pairs. Refer to Section 6.2.4 for the format of the Line Map files.

► To import a DXF-map or a Line Map

1. Right-click on any of the DXF File or Line Map File edit fields and select a file from a Map Files dialog box.
2. If necessary, use a scale factor to enlarge or reduce the appearance size of the map. Then use the values in X and Y to shift the scaled map to the desired position. For details, see Scaling a vector graphic in Section 2.102.

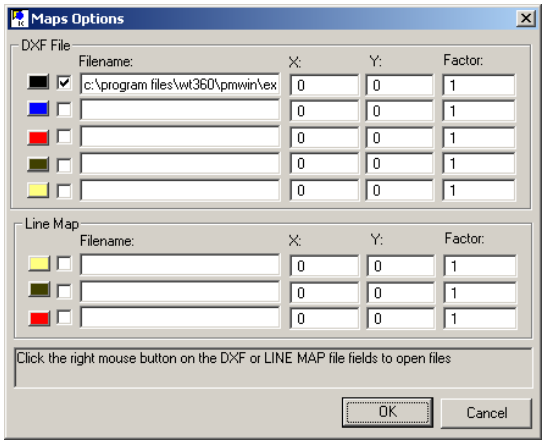


Fig. 3.15. The Maps Options dialog box

3. Click the colored button in the front of the edit field and select a color for the DXF-map from a Color dialog box. The color will be assigned to a DXF-graphics entity, if the entity's color is not defined in the DXF file. A line map will always use the selected color.
4. Check the check box next to the edit field. The map will be displayed only when the box is checked.

3.4 PMPATH Output Files

3.4.1 Plots

► To create plot files

1. Select *File* | *Save Plot As* to display the Save Plot As dialog box (Fig. 3.16).
2. Select a format from the Format drop-down box. The following five formats are available: Drawing Interchange Format (DXF), Hewlett Packard Graphics Language (HP-GL), MODPATH, PMPATH, and Windows Bitmap (BMP).
   If the MODPATH or PMPATH format is chosen, coordinates along the path of each particle are recorded in the file specified below. The file contains the starting coordinates of a particle, and the coordinates at every point where a particle leaves a cell (exit point). In addition, coordinates of intermediate points are saved whenever a particle tracking step length is reached. The saved files can be used by 3D Master [23] or 3D Groundwater Explorer [22] for advanced 3D visualization. Refer to Sections 6.2.11.2 and 6.2.11.1 for the format of the MODPATH and PMPATH files.
3. Type in the file name in the File edit field directly or right-click the edit field and select a file from a Plot File dialog box.
4. Click OK to save the file.
   Note that cross sectional plots can only be included in the DXF or BMP format. PMPATH uses the same color resolution as the video screen to capture and save Windows Bitmap files. A DXF-file is saved more compact and can be processed

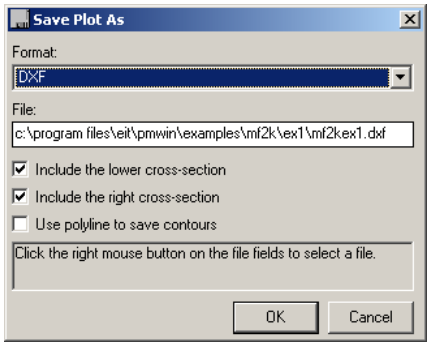


Fig. 3.16. The Save Plot As dialog box

by graphics software more efficiently, if the option "Use Polyline to save contours" is used. However, some graphics software packages do not support the POLYLINE feature. Use this feature only, if the user's graphics software package accepts the DXF entity POLYLINE.

3.4.2 Hydraulic Heads

Select *File* | *Save Heads As* to save the hydraulic head values of the current layer at the current stress period and time step in an ASCII Matrix file (see Section 6.2.1).

3.4.3 Drawdowns

Select *File* | *Save Heads As* to save the drawdown values of the current layer at the current stress period and time step in an ASCII Matrix file (see Section 6.2.1).

3.4.4 Flow Velocities

Select *File* | *Save Velocity As* and specify a file name in a File Save As dialog box to save flow velocities of the current layer at the current stress period and time step in an ASCII Matrix file (see Section 6.2.1). The file saves average pore velocities at the center of each cell. In addition, the velocity components along the I-, J- and K-axes are added to the end of the file. The default velocity at inactive cells is 1.0×10^{30}.

3.4.5 Particles

Select *File* | *Save Particles As* and specify a file name in a Save Particle As dialog box to save the particle position and attributes in a Particles file (see Section 6.2.12 for the format). By selecting a *Save as type* in this dialog box, either the starting position or end position (after backward or forward tracking) of the particles can be saved.

A Particles file can be loaded by selecting *File* | *Load Particles*. When a particle file is loaded, PMPATH just adds the additional particles to the model. Already existing particles will not be removed.

4

Tutorials

The tutorials provide an overview of the modeling process with **PM**, describe the basic skills you need to use **PM**, and take you step by step through hypothetical problems. Each tutorial is divided into three parts. It starts out with Folder, where you can find the ready-to-run model, for example *pmdir*\examples\tutorials \tutorial1\, where *pmdir* is the installation folder of **PM**. Next, you'll find a discussion of the hypothetical problem, and the step-by-step tutorial will walk you through the tasks.

4.1 Your First Groundwater Model with PM

Folder: *pmdir*\examples\tutorials\tutorial1

4.1.1 Overview of the Hypothetical Problem

It takes just a few minutes to build your first groundwater flow model with **PM**. First, create a groundwater model by choosing New Model from the File menu. Next, determine the size of the model grid by choosing Mesh Size from the Grid menu. Then, specify the geometry of the model and set the model parameters, such as hydraulic conductivity, effective porosity etc. Finally, perform the flow simulation by selecting *Models | MODFLOW | Run*.

After completing the flow simulation, you can use the modeling tools provided by **PM** to view the results, to calculate water budgets of particular zones, or graphically display the results, such as head contours. You can also use PMPATH to calculate and save path lines or use the finite difference transport models MT3DMS or MOC3D to simulate transport processes.

As shown in Fig. 4.1, an aquifer system with two stratigraphic units is bounded by no flow boundaries on the North and South sides. The West and East sides are bounded by rivers, which are in full hydraulic contact with the aquifer and can be considered as fixed head boundaries. The hydraulic heads on the west and east boundaries are 9 m and 8 m above reference level, respectively.

The aquifer system is unconfined and isotropic. The horizontal hydraulic conductivities of the first and second stratigraphic units are 0.0001 m/s and 0.0005 m/s, respectively. Vertical hydraulic conductivity of both units is assumed to be 10 percent of the horizontal hydraulic conductivity. The effective porosity is 25 percent. The elevation of the ground surface (top of the first stratigraphic unit) is 10m. The thickness of the first and the second units is 4 m and 6 m, respectively. A constant recharge rate of 8×10^{-9} m/s is applied to the aquifer. A contaminated area lies in the first unit next to the west boundary. The task is to isolate the contaminated area using a fully penetrating pumping well located next to the eastern boundary.

A numerical model has to be developed for this site to calculate the required pumping rate of the well. The pumping rate must be high enough so that the contaminated area lies within the capture zone of the pumping well. We will use **PM** to construct the numerical model and use PMPATH to compute the capture zone of the pumping well. Based on the calculated groundwater flow field, we will use MT3DMS to simulate the contaminant transport. We will show how to use PEST to calibrate the flow model and finally we will create an animation sequence displaying the development of the contaminant plume.

To demonstrate the use of the transport models, we assume that the contaminant is dissolved into groundwater at a rate of 1×10^{-4} $\mu g/s/m^2$. The longitudinal and transverse dispersivity values of the aquifer are 10 m and 1 m, respectively. The distribution coefficient for the linear equilibrium sorption is 0.000125. The bulk density of the porous medium is 2000 [kg/m^3]. The initial concentration, molecular diffusion coefficient, and decay rate are assumed to be zero. We will calculate the concentration distribution after a simulation time of 3 years and display the breakthrough curves (concentration-time series) at two points [X, Y] = [290, 310], [390, 310] in both units.

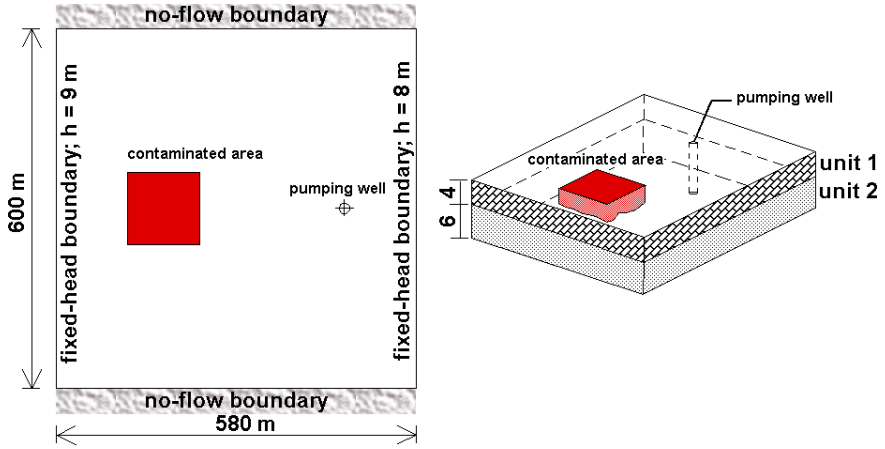


Fig. 4.1. Configuration of the hypothetical model

4.1.2 Run a Steady-State Flow Simulation

Six main steps must be performed in a steady-state flow simulation:

1. Create a new model
2. Assign model data
3. Perform the flow simulation
4. Check simulation results
5. Calculate subregional water budget
6. Produce output

4.1.2.1 Step 1: Create a New Model

The first step in running a flow simulation is to create a new model.

► To create a new model

1. Select *File* | *New Model*. A New Model dialog box appears. Select a folder for saving the model data, such as C:\Models\tutorial1, and type the file name TUTORIAL1 as the model name. A model must always have the file extension .PM5. All file names valid under MS-Windows with up to 120 characters can be used. It is a good idea to save every model in a separate folder, where the model and its output data will be kept. This will also allow **PM** to run several models simultaneously (multitasking).
2. Click *OK*.
   PM takes a few seconds to create the new model. The name of the new model name is shown in the title bar.

4.1.2.2 Step 2: Assign Model Data

The second step in running a flow simulation is to generate the model grid (mesh), specify cell status, and assign model parameters to the model grid.

PM requires the use of consistent units throughout the modeling process. For example, if you are using length $[L]$ units of meters and time $[T]$ units of seconds, hydraulic conductivity will be expressed in units of $[m/s]$, pumping rates will be in units of $[m^3/s]$ and dispersivities will be in units of $[m]$.

In MODFLOW, an aquifer system is replaced by a discretized domain consisting of an array of nodes and associated finite difference blocks (cells). Fig. 4.2 shows the spatial discretization scheme of an aquifer system with a mesh of cells and nodes at which hydraulic heads are calculated. The nodal grid forms the framework of the numerical model. Hydrostratigraphic units can be represented by one or more model layers. The thickness of each model cell and the width of each column and row may be variable. **PM** uses an index notation [Layer, Row, Column] for locating the cells. For example, the cell located in the first layer, 6th row, and 2nd column is denoted by [1, 6, 2]. In this example, the model domain is discretized in cells of horizontal dimensions of 20 m by 20 m. The first stratigraphic layer is represented by the first

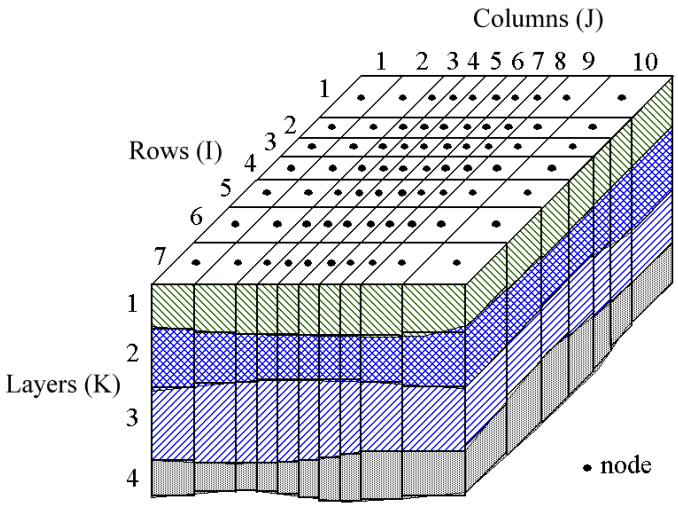


Fig. 4.2. The spatial discretization scheme and cell indices of MODFLOW

model layer and the second stratigraphic layer is represented by two model layers. It is to note that a higher resolution in the vertical direction is often required in order to correctly simulate the migration of contaminants.

► To generate the model grid

1. Select *Grid* | *Mesh Size*.
   The Model Dimension dialog box appears (Fig. 4.3).
2. Enter 3 for the number of layers, 10 for model thickness, 0 for the model top elevation, 30 for the numbers of rows and columns, 600 for the model extent in both row and column directions, and 10 for the vertical exaggeration.
   PM generates a uniform grid based on the specified dimensions. Later, the grid may be refined and the layer elevations can be adjusted. In this example, the first and second stratigraphic units will be represented by one and two model layers, respectively. Note that the model extent for the J Dimension is 600 m (instead of 580 m) because MODFLOW counts the distance between the center of the cells of the fixed-head boundaries.
3. Click *OK*. **PM** changes the pull-down menus and displays the generated model grid (Fig. 4.4). **PM** allows you to shift or rotate the model grid, change the width of each model column or row, or to add/delete model columns or rows. For this example, you do not need to modify the model grid. Refer to Section 2.1 for more information about the Grid Editor.
4. Select *File* | *Leave Editor* or click the leave editor button .

The next step is to specify the type of layers and the cell status array of the flow model. The cell status array (IBOUND array) contains a code for each model cell which indicates whether (1) the hydraulic head is computed (referred to as active

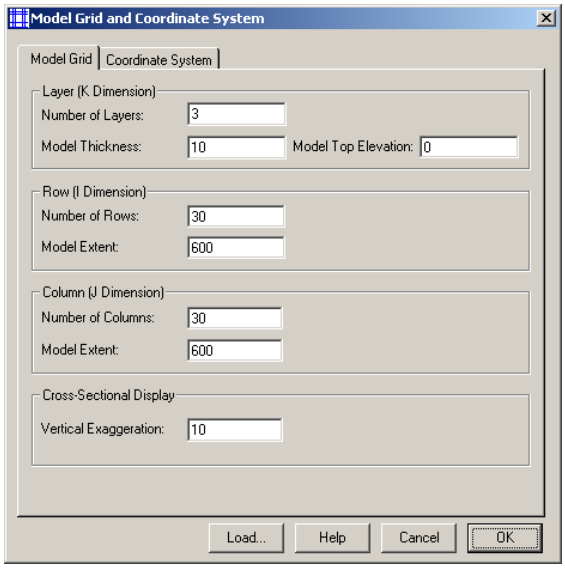


Fig. 4.3. The Model Dimension dialog box

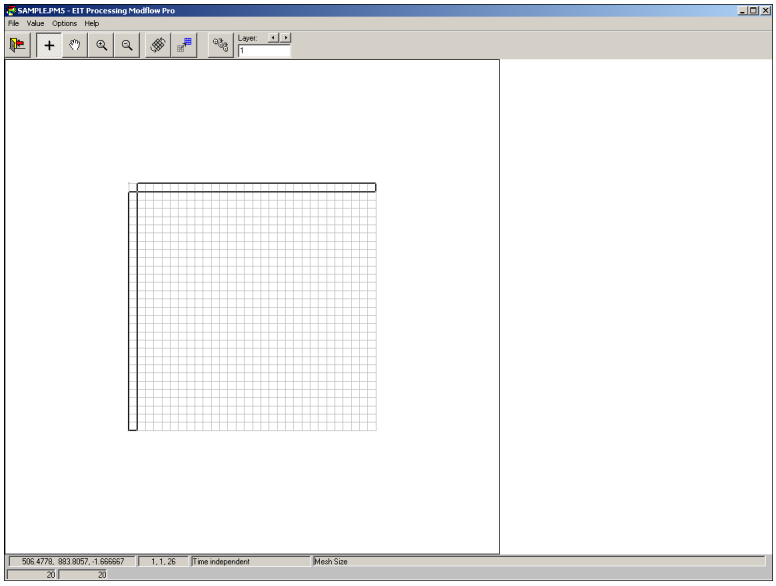


Fig. 4.4. The generated model grid

variable-head cell or active cell), (2) the hydraulic head is kept fixed at a given value (referred to as fixed-head cell, constant-head cell, or time-varying specified-head cell), or (3) no flow takes place within the cell (referred to as inactive cell). Use 1 for an active cell, -1 for a constant-head cell, and 0 for an inactive cell. For this example,

the value -1 needs to be assigned to the cells on the west and east boundaries and the value 1 to all other cells. Any outer boundary cell, which is not a constant-head cell, is automatically a zero flux boundary cell. Flux boundaries with non-zero fluxes are simulated by assigning appropriate infiltration or pumping wells in the corresponding active cell via the well package. Head-dependent boundary conditions are modeled on active cells by means of the general head boundary package or the river package.

► To define the layer properties

1. Select *Grid* | *Layer Property*.
   A Layer Options dialog box appears.
2. Click a cell of the Type column, a drop-down button will appear within the cell. By clicking the drop-down button, a list containing the available layer types (Fig. 4.5) will be displayed.
3. Select *1: Unconfined* for the first layer and *3: Confined/Unconfined* for the other layers then click OK to close the dialog box.

► To assign the cell status to the flow model

1. Select *Grid* | *Cell Status* | *IBOUND (Modflow)*. The Data Editor of **PM** appears and displays the model grid (Fig. 4.6). A *grid cursor* is located over the current cell. The value of the current cell is shown at the bottom of the status bar. The default value of the IBOUND array is 1. The grid cursor can be moved by using the arrow keys, by clicking the mouse on the desired position, or by using buttons in the tool bar. To jump to another layer, click the Layer edit box in the tool bar, type the new layer number, and then press enter.
   Note. A DXF-map is loaded by using the Maps Options dialog box. See Section 2.9.1 for details.

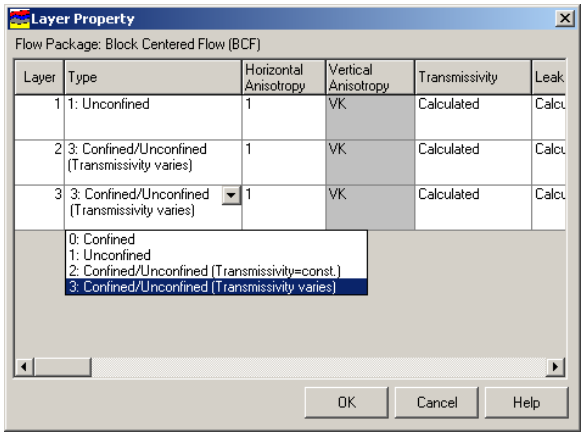


Fig. 4.5. The Layer Options dialog box and the layer type drop-down list

2. Move the grid cursor to the cell [1, 1, 1] and press the Enter key or the right mouse button to display a Cell Value dialog box.
3. Type -1 in the dialog box, then click OK.
   The upper-left cell of the model has been specified to be a constant-head cell.
4. Now turn on duplication by clicking the duplication button .
   Duplication is on, if the duplication button is depressed. The current cell value will be duplicated to all cells passed by the grid cursor, if it is moved while duplication is on. Duplication is turned off by clicking the duplication button again.
5. Move the grid cursor from the upper-left cell [1, 1, 1] to the lower-left cell [1, 30, 1] of the model grid.
   The value of -1 has now been duplicated to all cells on the west side of the model.
6. Move the grid cursor to the upper-right cell [1, 1, 30] by clicking on this cell.
7. Move the grid cursor from the upper-right cell [1, 1, 30] to the lower-right cell [1, 30, 30].
   The value of -1 has now been duplicated to all cells on the east side of the model.
8. Turn on layer copy by clicking the layer copy button .
   Layer copy is on, if the layer copy button is depressed. The cell values of the current layer will be copied to other layers, if model layer is changed while layer copy is on. Layer copy can be turned off by clicking the layer copy button again.
9. Move to the second layer and then to the third layer by pressing the PgDn key twice.
   The cell values of the first layer are copied to the second and third layers.
10. Select *File* | *Leave Editor* or click the leave editor button .

The next step is to specify the geometry of the model.

► To specify the elevation of the top of model layers

1. Select *Grid* | *Top of Layers (TOP)*.
   A Top of Layers (TOP) dialog box appears and asks if the layer bottom elevation should be used for the layer top elevation.
2. In the Top of Layers (TOP) dialog box, click No.
   PM displays the model grid.
3. Move the grid cursor to the first layer if it is not in the first layer.
4. Select *Value* | *Reset Matrix* (or press Ctrl+R).
   A Reset Matrix dialog box appears.
5. Enter 10 in the dialog box, then click OK.
   The elevation of the top of the first layer is set to 10.
6. Move to the second layer by pressing PgDn.
7. Repeat steps 3 and 4 to set the top elevation of the second layer to 6 and the top elevation of the third layer to 3.
8. Select *File* | *Leave Editor* or click the leave editor button .

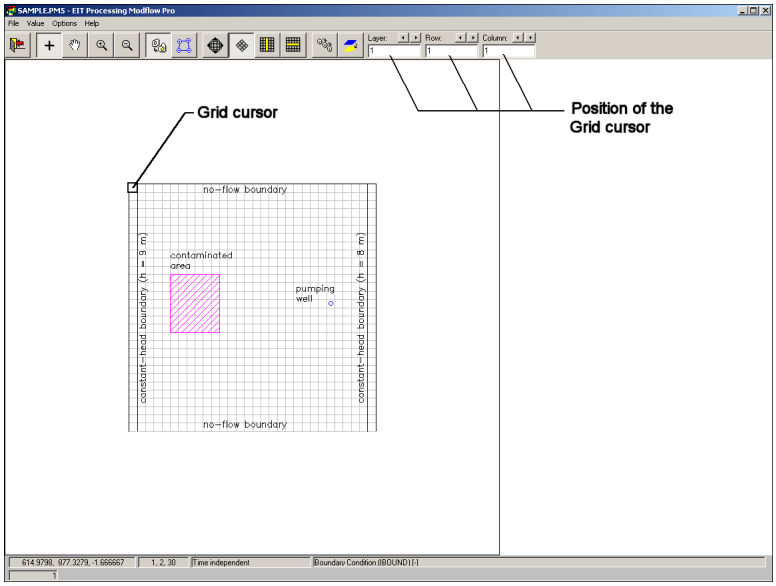


Fig. 4.6. The Data Editor displaying the plan view of the model grid

► To specify the elevation of the bottom of model layers

1. Select *Grid* | *Bottom of Layers (BOT)*.
2. Repeat the same procedure as described above to set the bottom elevation of the first, second and third layers to 6, 3 and 0, respectively.
3. Select *File* | *Leave Editor* or click the leave editor button .

We are going to specify the temporal and spatial parameters of the model. The spatial parameters for sample problem include the initial hydraulic head, horizontal and vertical hydraulic conductivities and effective porosity.

► To specify the temporal parameters

1. Select *Parameters* | *Time*.
   A Time Parameters dialog box appears. The temporal parameters include the time unit and the numbers of stress periods, time steps and transport steps. In MODFLOW, the simulation time is divided into stress periods - i.e., time intervals during which all external excitations or stresses are constant - which are, in turn, divided into time steps. Most transport models divide each flow time step further into smaller transport steps. The length of stress periods is not relevant to a steady state flow simulation. However, as we want to perform contaminant transport simulation, the actual time length must be specified in the table.
2. Enter 9.46728E+07 (seconds) for the Length of the first period.
3. Click *OK* to accept the other default values. This implies that a steady state flow simulation will be carried out.

Now, we need to specify the initial hydraulic head for each model cell. The initial hydraulic head at a constant-head boundary will be kept the same throughout the flow simulation. The other hydraulic head values are used as starting values in a transient simulation or first guesses for the iterative solver in a steady-state simulation. Here we firstly set all values to 8 and then correct the values on the west side by overwriting them with a value of 9.

► To specify the initial hydraulic head

1. Select *Parameters* | *Initial & Prescribed Hydraulic Heads* to display the model grid.
2. Move the grid cursor to the first layer.
3. Select *Value* | *Reset Matrix* (or press Ctrl+R) and enter 8 in the dialog box, then click OK.
4. Move the grid cursor to the cell [1, 1, 1] and press the Enter key or the right mouse button to display a Cell Value dialog box.
5. Enter 9 into the Cell Value dialog box, then click OK.
6. Now turn on duplication by clicking on the duplication button .
7. Move the grid cursor from the upper-left cell [1, 1, 1] to the lower-left cell [1, 30, 1] of the model grid. The value of 9 is duplicated to all cells on the west side of the model.
8. Turn on layer copy by clicking the layer copy button .
9. Move to the second layer and the third layer by pressing PgDn twice.
   The cell values of the first layer are copied to the second and third layers.
10. Select *File* | *Leave Editor* or click the leave editor button .

► To specify the horizontal hydraulic conductivity

1. Select *Parameters* | *Horizontal Hydraulic Conductivity*.
   PM displays the model grid.
2. Move the grid cursor to the first layer.
3. Select *Value* | *Reset Matrix* (or press Ctrl+R), enter 0.0001 in the dialog box, then click OK.
4. Move the grid cursor to the second layer.
5. Select *Value* | *Reset Matrix* (or press Ctrl+R), enter 0.0005 in the dialog box, then click OK.
6. Move the grid cursor to the third layer.
7. Select *Value* | *Reset Matrix* (or press Ctrl+R), enter 0.0005 in the dialog box, then click OK.
8. Select *File* | *Leave Editor* or click the leave editor button .

► To specify the vertical hydraulic conductivity

1. Select *Parameters* | *Vertical Hydraulic Conductivity*.
   PM displays the model grid.

2. Move the grid cursor to the first layer.
3. Select *Value* | *Reset Matrix* (or press Ctrl+R), enter 0.00001 in the dialog box, then click OK.
4. Move the grid cursor to the second layer.
5. Select *Value* | *Reset Matrix* (or press Ctrl+R), enter 0.00005 in the dialog box, then click OK.
6. Move the grid cursor to the third layer.
7. Select *Value* | *Reset Matrix* (or press Ctrl+R), enter 0.00005 in the dialog box, then click OK.
8. Select *File* | *Leave Editor* or click the leave editor button .

► To specify the effective porosity

1. Select *Parameters* | *Effective Porosity*.
   PM displays the model grid. Since the default value of 0.25 is the same as the prescribed value, nothing needs to be done here. Note that although a flow simulation does not require the effective porosity, it is necessary for the computation of travel times and contaminant transport processes.
2. Select *File* | *Leave Editor* or click the leave editor button .

► To specify the recharge rate

1. Select *Models* | *MODFLOW* | *Recharge*.
2. Select *Value* | *Reset Matrix* (or press Ctrl+R), enter 8E-9 for Recharge Flux $[L/T]$ in the dialog box, then click OK.
3. Select *File* | *Leave Editor* or click the leave editor button .

The last step before performing the flow simulation is to specify the location of the pumping well and its pumping rate. In MODFLOW, an injection or a pumping well is represented by a node (or a cell). The user specifies an injection or a pumping rate for each node. It is implicitly assumed that the well penetrates the full thickness of the cell. MODFLOW can simulate the effects of pumping from a well that penetrates more than one aquifer or layer provided that the user supplies the pumping rate for each layer. The total pumping rate for the multilayer well is equal to the sum of the pumping rates from the individual layers. The pumping rate for each layer (Q_k) can be approximately calculated by dividing the total pumping rate (Q_{total}) in proportion to the layer transmissivity (McDonald and Harbaugh 1988):

$$Q_k = Q_{total} \cdot \frac{T_k}{\Sigma T} \tag{4.1}$$

where T_k is the transmissivity of layer k and ΣT is the sum of the transmissivities of all layers penetrated by the multi-layer well. Unfortunately, as the first layer is unconfined, we do not exactly know the saturated thickness and the transmissivity of this layer at the position of the well. Equation 4.1 cannot be used unless we assume a

saturated thickness for calculating the transmissivity. Another possibility to simulate a multi-layer well is to set a very large vertical hydraulic conductivity (or vertical leakance), e.g. 1 m/s, to all cells of the well. The total pumping rate is assigned to the lowest cell of the well. For the display purpose, a very small pumping rate (say, $1 \times 10^{-10} m^3/s$) can be assigned to other cells of the well. In this way, the exact extraction rate from each penetrated layer will be calculated by MODFLOW implicitly and the value can be obtained by using the Water Budget Calculator (see below).

Since we do not know the required pumping rate for capturing the contaminated area shown in Fig. 4.1, we will try a total pumping rate of 0.0012 m^3/s.

► To specify the pumping well and the pumping rate

1. Select *Models* | *MODFLOW* | *Well*.
2. Move the grid cursor to the cell [1, 15, 25] and press the Enter key or the right mouse button to display a Cell Value dialog box.
3. Type -1E-10 in the dialog box, then click OK.
   Note that a negative value is used to indicate a pumping well.
4. Move the grid cursor to the cell [2, 15, 25] and press the Enter key or the right mouse button to display a Cell Value dialog box.
5. Type -1E-10 in the dialog box, then click OK.
6. Move the grid cursor to the cell [3, 15, 25] and press the Enter key or the right mouse button to display a Cell Value dialog box.
7. Type -0.0012 in the dialog box, then click OK.
8. Select *File* | *Leave Editor* or click the leave editor button .
9. Now select *Parameters* | *Vertical Hydraulic Conductivity* and change the vertical hydraulic conductivity value at the location of the well to 1 in all layers.

4.1.2.3 Step 3: Perform the Flow Simulation

Before starting the computation, a solver has to be chosen. This example uses the default solver PCG2 with its default settings. For details about the solvers, see Section 2.6.1.13.

► To perform the flow simulation

1. Select *Models* | *MODFLOW* | *Run*
   The Run Modflow dialog box appears (Fig. 4.7).
2. Click *OK* to start the flow simulation.
   Prior to running MODFLOW, **PM** will use the user-specified data to generate input files for MODFLOW (and optionally MODPATH) as listed in the table of the Run Modflow dialog box. An input file will be generated only if its generate flag is set to ☑. Normally, the flags do not need to be changed, since **PM** will take care of the settings automatically. If necessary, click on the check box to toggle the generate flag between ☑ and ☐.

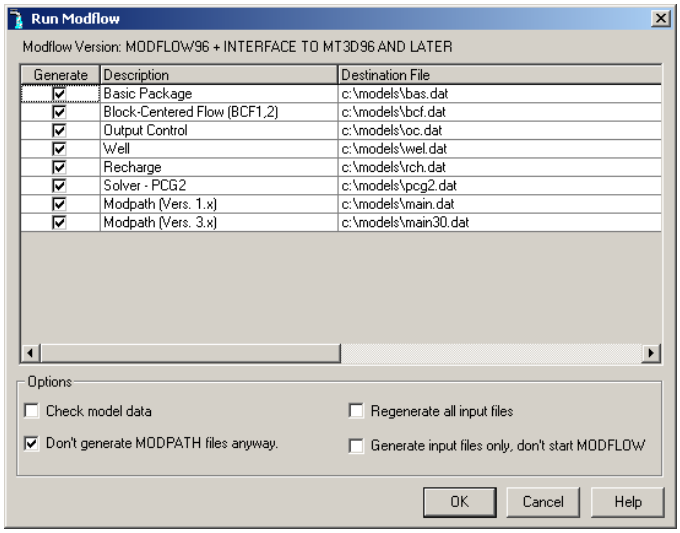


Fig. 4.7. The Run Modflow dialog box

4.1.2.4 Step 4: Check Simulation Results

During a flow simulation, MODFLOW writes a detailed run record to *path*\OUTPUT.DAT, where *path* is the folder in which the model data are saved. When a flow simulation is completed successfully, MODFLOW saves the simulation results in various unformatted (binary) files as listed in Table 4.1. Prior to running MODFLOW, the user may control the output of these unformatted (binary) files by choosing *Models* | *MODFLOW* | *Output Control*. The output file path\INTERBED.DAT will only be generated, if the Interbed Storage Package is activated (see Chapter 2 for details about the Interbed Storage Package).

The system of equations of the finite difference model MODFLOW actually consists of a flow continuity statement for each model cell. Since MODFLOW uses iterative equation solvers, the accuracy of the simulation results need to be checked after each simulation run. Continuity should exist for the total flows into and out of the entire model or any sub-region of the model. This means that the difference between total inflow and total outflow should theoretically equal to 0 for a steady-state flow simulation or equal to the total change in storage for a transient flow simulation. To verify the accuracy of the results, MODFLOW calculates a volumetric water budget for the entire model at the end of each time step, and saves it in the listing file output.dat (see Table 4.2). The water budget provides an indication of the overall acceptability of the numerical solution. If the accuracy is insufficient, a new run should be made using a smaller convergence criterion in the iterative solver (see Section 2.6.1.13). It is recommended to check the listing file by selecting *Models* | *MODFLOW* | *View* | *Run Listing File*. This file contains other further essential information. In case of difficulties, this supplementary information could be very helpful.

Table 4.1 Output files from MODFLOW

File	Contents
path\OUTPUT.DAT	Detailed run record and simulation report
path\HEADS.DAT	Hydraulic heads
path\DDOWN.DAT	Drawdowns, the difference between the starting heads and the calculated hydraulic heads.
path\BUDGET.DAT	Cell-by-Cell flow terms.
path\INTERBED.DAT	Subsidence of the entire aquifer and compaction and preconsolidation heads in individual layers.
path\MT3D.FLO	Interface file to MT3D/MT3DMS. This file is created by the LKMT package provided by MT3D/MT3DMS (Zheng 1990, 1998).

- *path* is the folder in which the model data are saved.

Table 4.2 Volumetric budget for the entire model written by MODFLOW

```
     CUMULATIVE VOLUMES      L**3       RATES FOR THIS TIME STEP      L**3/T
     ------------------                 ------------------------

           IN:                                   IN:
           ---                                   ---
     CONSTANT HEAD =      209924.1410     CONSTANT HEAD =       2.2174E-03
             WELLS =           0.0000             WELLS =           0.0000
          RECHARGE =      254170.0160          RECHARGE =       2.6848E-03
          TOTAL IN =      464094.1560          TOTAL IN =       4.9022E-03

          OUT:                                  OUT:
          ----                                  ----
     CONSTANT HEAD =      350429.7810     CONSTANT HEAD =       3.7016E-03
             WELLS =      113604.0160             WELLS =       1.2000E-03
          RECHARGE =           0.0000          RECHARGE =           0.0000
         TOTAL OUT =      464033.8130         TOTAL OUT =       4.9016E-03
          IN - OUT =          60.3438          IN - OUT =       6.3796E-07
PERCENT DISCREPANCY =            0.01 PERCENT DISCREPANCY =           0.01
```

4.1.2.5 Step 5: Calculate subregional water budget

There are situations in which it is useful to calculate water budgets for various subregions of the model. To facilitate such calculations, flow terms for individual cells are saved in the file path\BUDGET.DAT. These individual cell flows are referred to as cell-by-cell flow terms, and are of four types:

1. cell-by-cell stress flows, or flows into or from an individual cell due to one of the external stresses (excitations) represented in the model, e.g., pumping well or recharge;
2. cell-by-cell storage terms, which give the rate of accumulation or depletion of storage in an individual cell;
3. cell-by-cell constant-head flow terms, which give the net flow to or from individual fixed-head cells; and
4. internal cell-by-cell flows, which are the flows across individual cell faces-that is, between adjacent model cells. The Water Budget Calculator uses the cell-by-cell flow terms to compute water budgets for the entire model, user-specified sub regions, and flows between adjacent sub regions.

► To calculate subregional water budget

1. Select *Tools* | *Water Budget*.
   The Water Budget dialog box appears (Fig. 4.8).
2. Click *Subregions*.
   PM displays the model grid. Click the button if the display mode is not Grid View. The water budget of each subregion will be calculated. A subregion is indicated by a number ranging from 0 to 50. A number must be assigned to each model cell. The number 0 indicates that a cell is not associated with any subregion. Follow the steps below to assign subregion numbers 1 to the first and 2 to the second layer.
3. Move the grid cursor to the first layer.
4. Select *Value* | *Reset Matrix*, type 1 in the Reset Matrix dialog box, then click OK.
5. Move the grid cursor to the second layer by pressing the PgDn key.
6. Select *Value* | *Reset Matrix*, type 2 in the Reset Matrix dialog box, then click OK.
7. Select *File* | *Leave Editor* or click the leave editor button .
8. Click *OK* in the Water Budget dialog box.

PM calculates and saves the flows in the file path\WATERBDG.DAT as shown in Table 4.3. The unit of the flows is $[L^3T^{-1}]$. Flows are calculated for each subregion in each layer and each time step. Flows are considered as IN, if they are entering a subregion. Flows between subregions are given in a Flow Matrix. *HORIZ. EXCHANGE* gives the flow rate horizontally across the boundary of a zone. *EXCHANGE (UPPER)* gives the flow rate coming from (IN) or going to (OUT) to the upper adjacent layer. *EXCHANGE (LOWER)* gives the flow rate coming from (IN) or going to (OUT) to the lower adjacent layer. For example, the flow rate from the first layer to the second layer (2.6107365E-03 m^3/s) is saved in EXCHANGE (LOWER) of REGION = 1 and LAYER = 1.

The percent discrepancy in Table 4.3 is calculated by

$$\frac{100 \cdot (IN - OUT)}{(IN + OUT)/2} \tag{4.2}$$

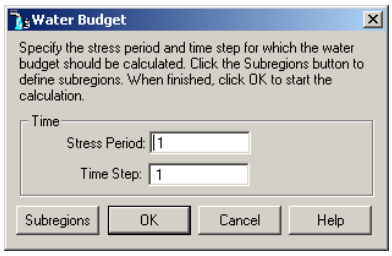

Water Budget
Specify the stress period and time step for which the water budget should be calculated. Click the Subregions button to define subregions. When finished, click OK to start the calculation.
Time
Stress Period: 1
Time Step: 1
Subregions
OK
Cancel
Help

Fig. 4.8. The Water Budget dialog box

Table 4.3 Output from the Water Budget Calculator

```
============================================================
 WATER BUDGET OF SUBREGIONS WITHIN EACH INDIVIDUAL LAYER
============================================================
 REGION   1  IN LAYER   1
------------------------------------------------
       FLOW TERM             IN             OUT         IN-OUT
         STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
   CONSTANT HEAD  1.8595711E-04  2.4354266E-04 -5.7585552E-05
 HORIZ. EXCHANGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
EXCHANGE (UPPER)  0.0000000E+00  0.0000000E+00  0.0000000E+00
EXCHANGE (LOWER)  0.0000000E+00  2.6107365E-03 -2.6107365E-03
           WELLS  0.0000000E+00  1.0000000E-10 -1.0000000E-10
          DRAINS  0.0000000E+00  0.0000000E+00  0.0000000E+00
        RECHARGE  2.6880163E-03  0.0000000E+00  2.6880163E-03
               .              .              .              .
               .              .              .              .
SUM OF THE LAYER  2.8739735E-03  2.8542792E-03  1.9694213E-05
 DISCREPANCY [%]  0.69
               .              .              .              .
               .              .              .              .
 REGION   2  IN LAYER   2
------------------------------------------------
       FLOW TERM             IN             OUT         IN-OUT
         STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
   CONSTANT HEAD  1.0105607E-03  1.7374435E-03 -7.2688283E-04
 HORIZ. EXCHANGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
EXCHANGE (UPPER)  2.6107365E-03  0.0000000E+00  2.6107365E-03
EXCHANGE (LOWER)  0.0000000E+00  1.9322647E-03 -1.9322647E-03
           WELLS  0.0000000E+00  1.0000000E-10 -1.0000000E-10
          DRAINS  0.0000000E+00  0.0000000E+00  0.0000000E+00
        RECHARGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
               .              .              .              .
               .              .              .              .
SUM OF THE LAYER  3.6212972E-03  3.6697080E-03 -4.8410846E-05
 DISCREPANCY [%] -1.33
               .              .              .              .
               .              .              .              .
============================================================
WATER BUDGET OF THE WHOLE MODEL DOMAIN:
============================================================
         STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
   CONSTANT HEAD  2.2167889E-03  3.7117251E-03 -1.4949362E-03
           WELLS  0.0000000E+00  1.2000003E-03 -1.2000003E-03
          DRAINS  0.0000000E+00  0.0000000E+00  0.0000000E+00
        RECHARGE  2.6880163E-03  0.0000000E+00  2.6880163E-03
               .              .              .              .
               .              .              .              .
------------------------------------------------------------
             SUM  4.9048052E-03  4.9117254E-03 -6.9201924E-06
 DISCREPANCY [%] -0.14

============================================================
FLOW RATES BETWEEN SUBREGIONS
============================================================
The value of the element (i,j) of the following flow
matrix gives the flow rate from the i-th region to
the j-th region. Where i is the column index and j is
the row index.

FLOW MATRIX:
           1           2           3
.....................................
  1    0.000       0.000       0.000
  2   2.6107E-03   0.000       0.000
  3    0.000      1.9323E-03   0.000
```

In this example, the percent discrepancy of in- and outflows for the model and each zone in each layer is acceptably small. This means the model equations have been correctly solved.

To calculate the exact flow rates to the well, we repeat the previous procedure for calculating subregional water budgets. This time we only assign the cell [1, 15, 25] to zone 1, the cell [2, 15, 25] to zone 2 and the cell [3, 15, 25] to zone 3. All other cells are assigned to zone 0. The water budget is shown in Table 4.4. The pumping well

Table 4.4 Output from the Water Budget Calculator for the pumping well

```
FLOWS ARE CONSIDERED ''IN'' IF THEY ARE ENTERING A SUBREGION
THE UNIT OF THE FLOWS IS [L^3/T]
 ============================================================
  WATER BUDGET OF SUBREGIONS WITHIN EACH INDIVIDUAL LAYER
 ============================================================
  REGION   1  IN LAYER   1
 ------------------------------------------------
        FLOW TERM             IN            OUT         IN-OUT
          STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
    CONSTANT HEAD  0.0000000E+00  0.0000000E+00  0.0000000E+00
   HORIZ. EXCHANGE  7.8003708E-05  0.0000000E+00  7.8003708E-05
  EXCHANGE (UPPER)  0.0000000E+00  0.0000000E+00  0.0000000E+00
  EXCHANGE (LOWER)  0.0000000E+00  7.9934180E-05 -7.9934180E-05
            WELLS  0.0000000E+00  1.0000000E-10 -1.0000000E-10
           DRAINS  0.0000000E+00  0.0000000E+00  0.0000000E+00
         RECHARGE  3.1999998E-06  0.0000000E+00  3.1999998E-06
                .             .             .             .
                .             .             .             .
  SUM OF THE LAYER  8.1203711E-05  7.9934282E-05  1.2694290E-06
                .             .             .             .
                .             .             .             .
  REGION   2  IN LAYER   2
 ------------------------------------------------
        FLOW TERM             IN            OUT         IN-OUT
          STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
    CONSTANT HEAD  0.0000000E+00  0.0000000E+00  0.0000000E+00
   HORIZ. EXCHANGE  5.6002894E-04  0.0000000E+00  5.6002894E-04
  EXCHANGE (UPPER)  7.9934180E-05  0.0000000E+00  7.9934180E-05
  EXCHANGE (LOWER)  0.0000000E+00  6.3981197E-04 -6.3981197E-04
            WELLS  0.0000000E+00  1.0000000E-10 -1.0000000E-10
                .             .             .             .
                .             .             .             .
  SUM OF THE LAYER  6.3996314E-04  6.3981209E-04  1.5104888E-07
                .             .             .             .
                .             .             .             .
  REGION   3  IN LAYER   3
 ------------------------------------------------
        FLOW TERM             IN            OUT         IN-OUT
          STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
    CONSTANT HEAD  0.0000000E+00  0.0000000E+00  0.0000000E+00
   HORIZ. EXCHANGE  5.5900711E-04  0.0000000E+00  5.5900711E-04
  EXCHANGE (UPPER)  6.3981197E-04  0.0000000E+00  6.3981197E-04
  EXCHANGE (LOWER)  0.0000000E+00  0.0000000E+00  0.0000000E+00
            WELLS  0.0000000E+00  1.2000001E-03 -1.2000001E-03
                .             .             .             .
                .             .             .             .
  SUM OF THE LAYER  1.1988191E-03  1.2000001E-03 -1.1809170E-06
```

is abstracting 7.8003708E-05 m^3/s from the first layer, 5.6002894E-04 m^3/s from the second layer and 5.5900711E-04 m^3/s from the third layer. Almost all water withdrawn comes from the second stratigraphic unit, as can be expected from the configuration of the aquifer.

4.1.2.6 Step 6: Produce Output

In addition to the water budget, **PM** provides various possibilities for checking simulation results and creating graphical outputs. The particle-tracking model PMPATH can display pathlines, head and drawdown contours, and velocity vectors. Using the Results Extractor, simulation results of any layer and time step can be read from the unformatted (binary) result files and saved in ASCII Matrix files. An ASCII Matrix file contains a value for each model cell in a layer. **PM** can load ASCII matrix files into a model grid. The format of the ASCII Matrix file is described in Section 6.2.1. **PM** includes a built-in 2D visualization tool, which can be used to display contours of almost all kind of model results, including hydraulic heads, drawdown, concen-

tration, and other values.

We will carry out the following tasks in this step:

1. Use the Results Extractor to read and save the calculated hydraulic heads.
2. Create a contour map based on the calculated hydraulic heads.
3. Use PMPATH to compute pathlines as well as the capture zone of the pumping well.

► To read and save the calculated hydraulic heads

1. Select *Tools* | *Results Extractor*.
   The Results Extractor dialog box appears (Fig. 4.9). The options in the Results Extractor dialog box are grouped under six tabs - MODFLOW, MOC3D, MT3D, MT3DMS, and RT3D. In the MODFLOW tab, you may choose a result type from the Result Type drop down box. You may specify the layer, stress period and time step from which the result should be read. The spreadsheet displays a series of columns and rows. The intersection of a row and column is a cell. Each cell of the spreadsheet corresponds to a model cell in a layer. Refer to Section 2.7.6 for details about the Results Extractor. For the current sample problem, follow steps 2 to 6 to save the hydraulic heads of each layer in three ASCII Matrix files.
2. Choose *Hydraulic Head* from the *Result Type* drop down box.
3. Type 1 in the *Layer* edit field. For this example (steady-state flow simulation with only one stress period and one time step), the stress period and time step number should be 1.

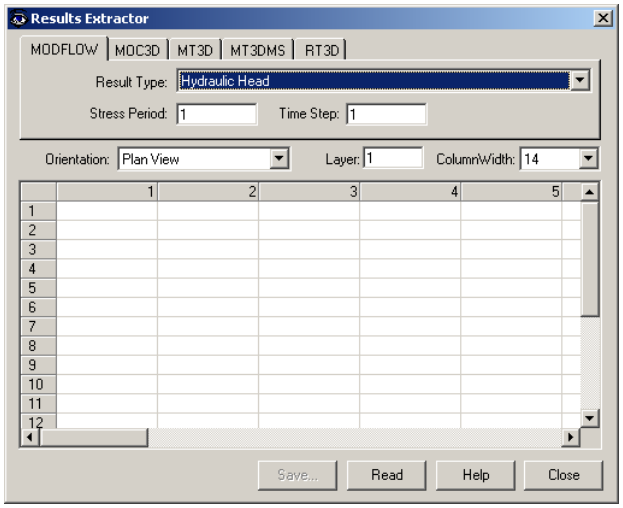


Fig. 4.9. The Results Extractor dialog box

4. Click *Read*. Hydraulic heads in the first layer at time step 1 and stress period 1 will be read and put into the spreadsheet. You can scroll the spreadsheet by clicking on the scrolling bars next to the spreadsheet.
5. Click *Save*. A Save Matrix As dialog box appears. By setting the Save as type option, the result can be optionally saved as an ASCII matrix or a SURFER data file. Specify the file name H1.DAT and select a folder in which H1.DAT should be saved. Click OK when ready.
6. Repeat steps 3, 4 and 5 to save the hydraulic heads of the second and third layer in the files H2.DAT and H3.DAT, respectively.
7. Click Close to close the dialog box.

► To generate contour maps of the calculated heads

1. Select *Tools* | *2D Visualization*.
   The Result Selection dialog box (Fig. 4.10) appears.
2. Click *OK* to select the default result type *Hydraulic Head*.
   PM displays the model grid and head contours (Fig. 4.11). By default, **PM** sets 10 contour levels ranging from the minimum to the maximum value. One can customize the appearance of the contour lines by using the Environment Options dialog box. Refer to Section 2.9.2 for details about this dialog box.
3. To save or print the graphics, select *File* | *Save Plot As* or *File* | *Print Plot*.
4. Select *File* | *Leave Editor* or click the leave editor button .

► To draw a pathline

1. Select *Models* | *PMPATH (Pathlines and Contours)* if PMPATH is not yet started.
   PM calls the advective transport model PMPATH, which will load the current model automatically. PMPATH uses a grid cursor to define the column and row for which the cross sectional plots should be displayed. You can move the grid cursor by holding down the Ctrl key and click the left mouse button on the desired position. ***Note.*** If you subsequently modify and calculate a model within **PM**, you must load the modified model into PMPATH again to ensure that the modifications can be recognized by PMPATH. To load a model, click and select a model file with the extension .PM5 from the Open Model dialog box.
2. Click the Set Particle button .
3. Right-click on a point within the model area to set a particle.

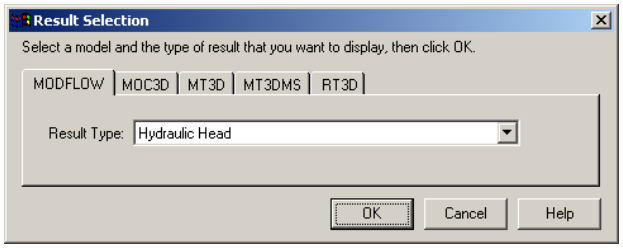


Fig. 4.10. The Result Selection dialog box

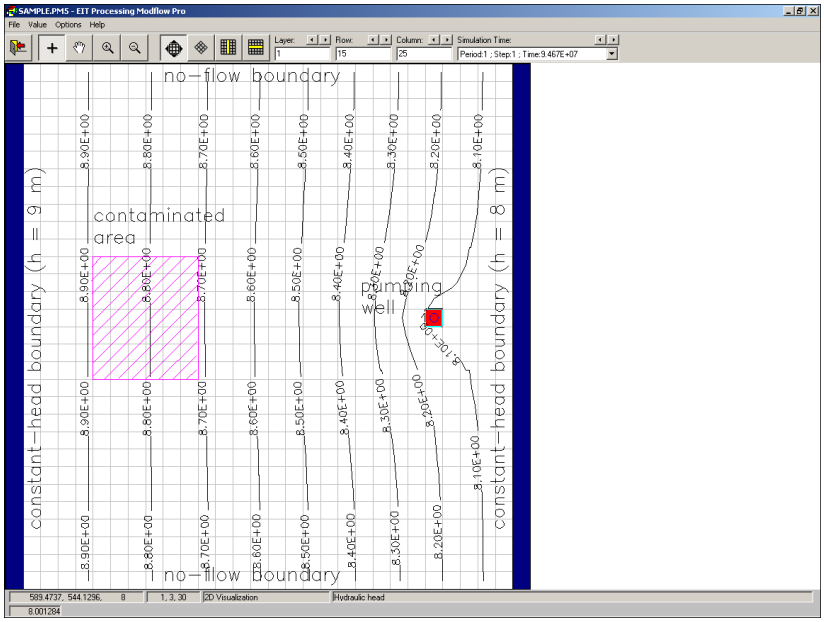


Fig. 4.11. Contours of the hydraulic heads in the first layer

4. Click ◄ to start the backward particle tracking.
5. Click ► to start the forward particle tracking.
   Each time you press one of the buttons ◄| or |►, particle(s) may move back-ward or forward for a defined time length. Refer to Section 3.3.2 for the definition of the time length.

► To delineate the capture zone of the pumping well

1. Select *Models* | *PMPATH (Pathlines and Contours)* if PMPATH is not yet started.
2. Click the Set Particle button +.
3. Move the mouse pointer to the model area. The mouse pointer turns into crosshairs.
4. Place the crosshairs at the upper-left corner of the pumping well, as shown in Fig. 4.12
5. Hold down the left mouse button and drag the crosshairs until the window covers the pumping well.
6. Release the left mouse button.
   An Add New Particles dialog box appears. Assign the numbers of particles to the edit fields in the dialog box as shown in Fig. 4.13. Click the Properties tab and click the colored button to select an appropriate color for the new particles. When finished, click OK.

7. To set particles around the pumping well in the second and third layer, press PgDn to move down a layer and repeat steps 4 through 6. Use other colors for the new particles in the second and third layers.
8. Click to start the backward particle tracking.
   PMPATH calculates and shows the projections of the pathlines as well as the capture zone of the pumping well (Fig. 4.14).

To see the projection of the path lines on the cross section windows in greater details, open an Environment Options dialog box by selecting *Options* | *Environment* and setting a larger exaggeration value for the vertical scale in the Cross Sections tab. Fig. 4.15 shows the same path lines by setting the vertical exaggeration value to 10. Note that some path lines end up at the groundwater surface, where recharge occurs. This is one of the major differences between a three-dimensional and a two-dimensional model. In two-dimensional simulation models, such as ASM for Windows [20], FINEM [70] or MOC [73], a vertical velocity term does not exist (or always equals to zero). This leads to the result that path lines can never be tracked back to the ground surface where the groundwater recharge from the precipitation occurs. Note that pathlines can be drawn in 3 dimensions in PMPATH even if you build a 2D model. See Section 5.1.1 for an example.

PMPATH can create time-related capture zones of pumping wells. The 100-days-capture zone shown in Fig. 4.16 is created using the settings in the Particle Tracking (Time) Properties dialog box (Fig. 4.17) and clicking . To open this dialog box, select *Options* | *Particle Tracking (Time)*. Refer to Section 3.3.2 for details about this

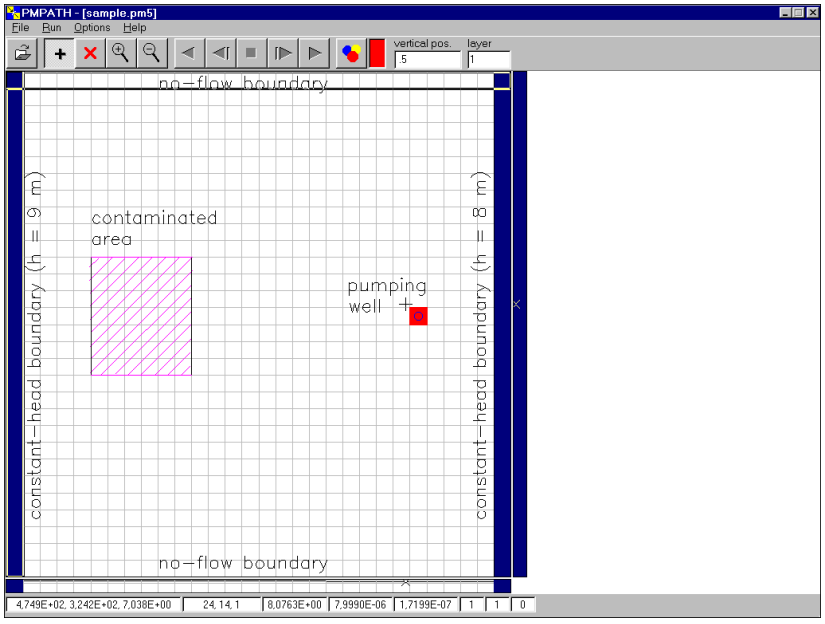


Fig. 4.12. The model loaded in PMPATH

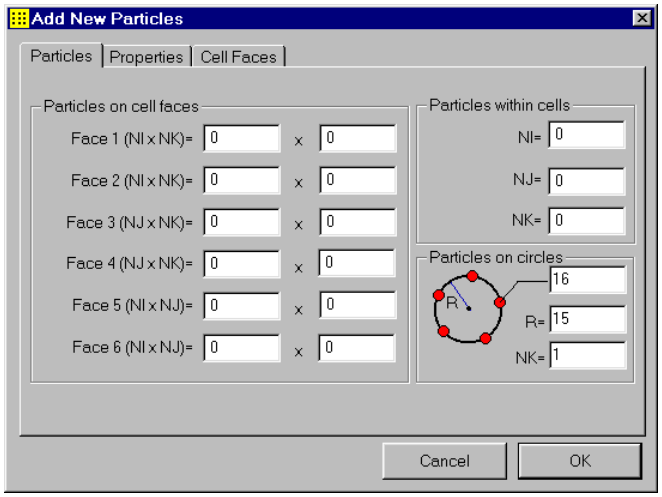


Fig. 4.13. The Add New Particles dialog box

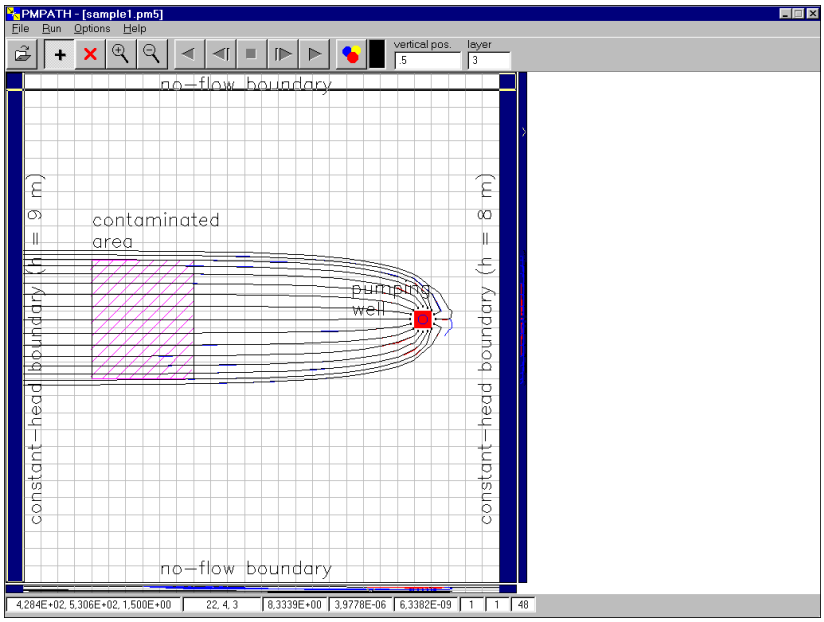


Fig. 4.14. The capture zone of the pumping well (vertical exaggeration = 1)

dialog box. Note that the capture zone in the first layer is smaller than those in the other layers due to lower hydraulic conductivity (and thus lower flow velocity) of the first layer.

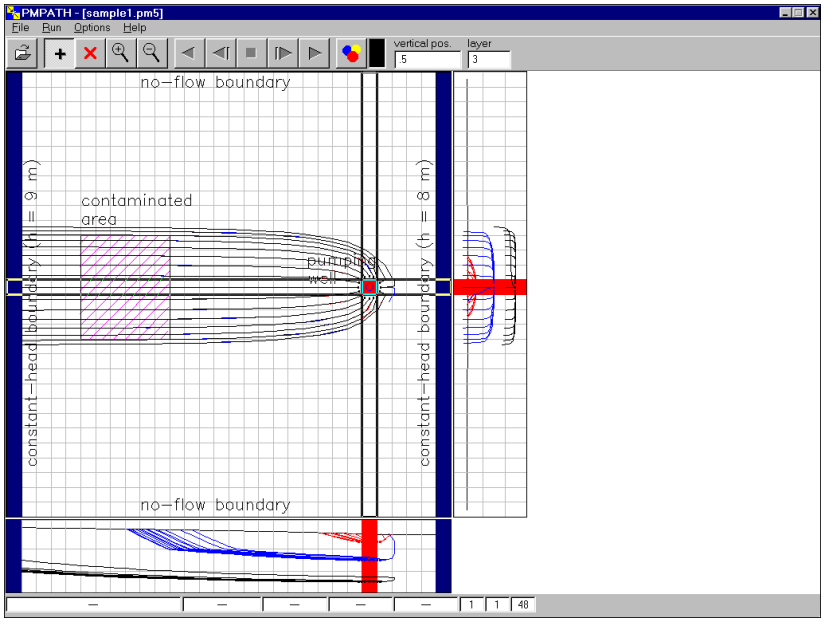


Fig. 4.15. The capture zone of the pumping well (vertical exaggeration = 10)

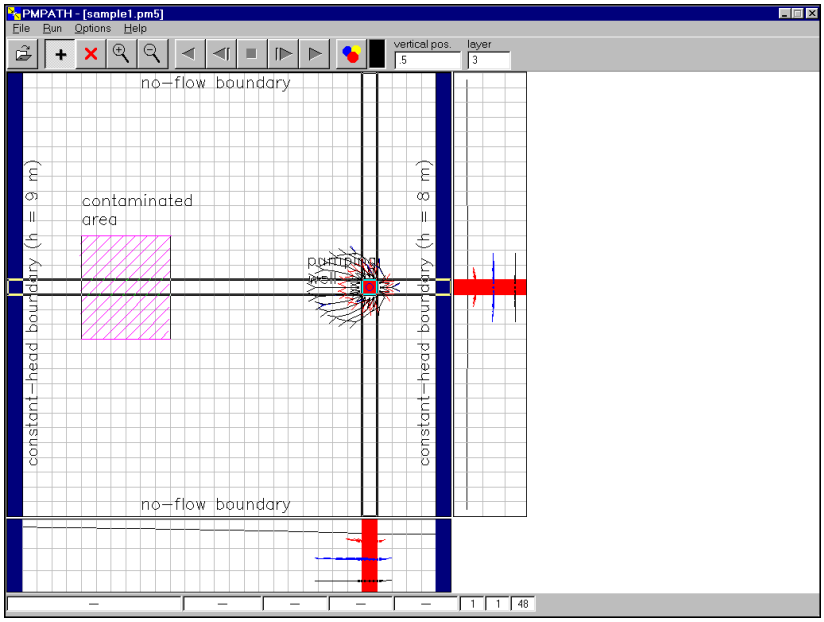


Fig. 4.16. The 100-day capture zone calculated by PMPATH

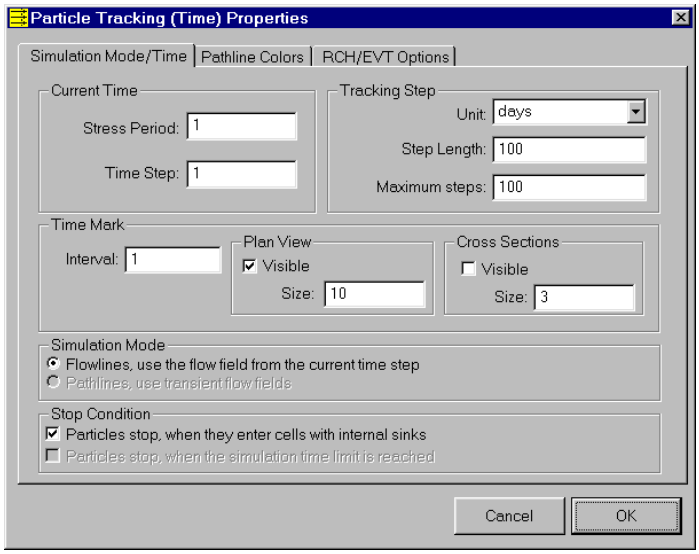


Fig. 4.17. The Particle Tracking (Time) Properties dialog box

4.1.3 Simulation of Solute Transport

Basically, the transport of solutes in porous media can be described by three processes: advection, hydrodynamic dispersion and physical, chemical or biochemical reactions. The MT3DMS and MOC3D models use the method-of-characteristics (MOC) to simulate the advective transport, in which dissolved chemicals are represented by a number of particles and the particles are moving with the flowing groundwater. Besides the MOC method, the MT3DMS model provide several other methods for solving the advective term, see Section 2.6.2.3 for details.

The hydrodynamic dispersion can be expressed in terms of the dispersivity $[L]$ and the coefficient of molecular diffusion $[L^2T^{-1}]$ for the solute in the porous medium. The types of reactions incorporated into MOC3D are restricted to those that can be represented by a first-order rate reaction, such as radioactive decay, or by a retardation factor, such as instantaneous, reversible, sorption-desorption reactions governed by a linear isotherm and constant distribution coefficient (K_d). In addition to the linear isotherm, MT3DMS supports non-linear isotherms, i.e., Freundlich and Langmuir isotherms.

Prior to running MT3DMS or MOC3D, you need to define the observation boreholes, for which the breakthrough curves will be calculated.

► To define observation boreholes

1. Select *Models* | *MT3DMS* | *Concentration Observations* or *Models* | *MOC3D* | *Concentration Observations* A Concentration Observation dialog box appears. Enter the coordinates of the observation boreholes into the dialog box as shown in Fig. 4.18. For boreholes 1 and 2, set the proportion value of the first layer to

1 and other layers to 0. This means that these two boreholes are screened at the first layer. For boreholes 3 and 4, set the proportion value of the second layer to 1 and other layers to 0. For boreholes 5 and 6, set the proportion value of the third layer to 1 and other layers to 0.

2. Click *OK* to close the dialog box.

4.1.3.1 Perform Transport Simulation with MT3DMS

MT3DMS requires a cell status code for each model cell, which indicates whether (1) solute concentration varies with time (active concentration cell), (2) the concentration is kept fixed at a constant value (constant-concentration cell), or (3) the cell is an inactive concentration cell. Use 1 for an active concentration cell, -1 for a constant-concentration cell, and 0 for an inactive concentration cell. Active, variable-head cells can be treated as inactive concentration cells to minimize the area needed for transport simulation, as long as the solute concentration is insignificant near those cells.

Similar to the flow model, you must specify the initial concentration for each model cell. The initial concentration value at a constant-concentration cell will be kept constant during a transport simulation. The other concentration values are used as starting values in a transport simulation.

► To assign the cell status to MT3DMS

1. Select *Grid* | *Cell Status* | *ICBUND (MT3D/MT3DMS)*.
   For the current example, we accept the default value 1 for all cells.

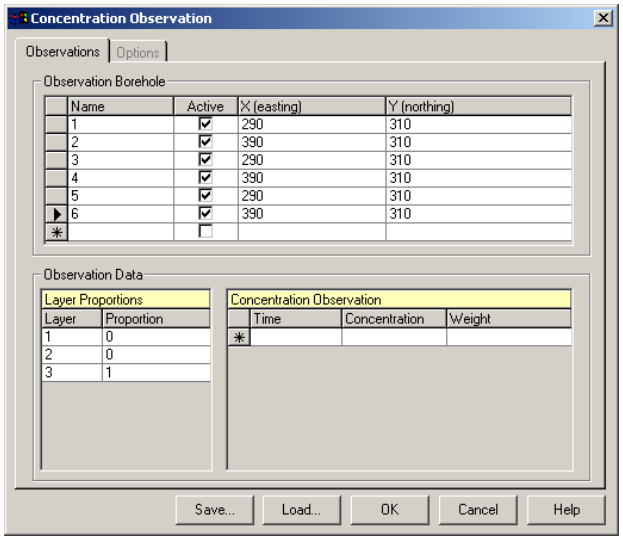


Fig. 4.18. The Concentration Observation dialog box

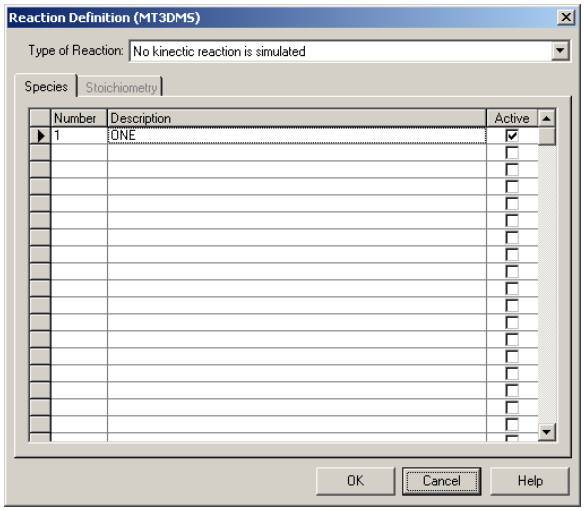


Fig. 4.19. The Reaction Definition dialog box

2. Select *File* | *Leave Editor* or click the leave editor button .

Since MT3DMS is capable of handling multiple species, we need to define the number of species involved in the simulation. This is done by defining the reaction types and species in the following steps.

► To set reaction definition

1. Select *Models* | *MT3DMS* | *Reaction Definition*.
   The Reaction Definition dialog box (Fig. 4.19) appears.
2. In the Reaction Definition dialog box, set the *Type of Reaction* to "No kinetic reaction is simulated", and activate the first species by checking the Active box of the first row of the table. Modify the description of the species as needed.
3. Click *OK* to close the dialog box.

► To set the initial concentration

1. Select *Models* | *MT3DMS* | *Initial Concentration*.
   For the current example, we accept the default value 0 for all cells.
2. Select *File* | *Leave Editor* or click the leave editor button .

► To assign the input rate of contaminants

1. Select *Models* | *MT3DMS* | *Sink/Source Concentration* | *Recharge*.
2. Assign 12500 [$\mu g/m^3$] to the cells within the contaminated area.
   This value is the concentration associated with the recharge flux. Since the recharge rate is 8×10^{-9} [$m^3/m^2/s$] and the dissolution rate is 1×10^{-4}

$[\mu g/s/m^2]$, the concentration associated with the recharge flux is $1 \times 10^{-4}/8 \times 10^{-9} = 12500$ $[\mu g/m^3]$.

3. Select *File* | *Leave Editor* or click the leave editor button .

► To assign the transport parameters to the Advection Package

1. Select *Models* | *MT3DMS* | *Advection*.
   The Advection Package (MT3DMS) dialog box appears. Enter the values shown in Fig. 4.20 into the dialog box, select Method of Characteristics (MOC) for the solution scheme, and First-order Euler for the particle-tracking algorithm.
2. Click *OK* to close the dialog box.

► To assign the dispersion parameters

1. Select *Models* | *MT3DMS* | *Dispersion*.
   The Dispersion Package (MT3D) dialog box appears. Enter the ratios of the transverse dispersivity to longitudinal dispersivity as shown in Fig. 4.21.
2. Click *OK*. **PM** displays the model grid. At this point you need to specify the longitudinal dispersivity to each cell of the grid.
3. Click the button if the display mode is not Grid View.
4. Select *Value* | *Reset Matrix* (or press Ctrl+R), type 10 in the dialog box, and select the option *Apply to the entire model* then click OK to assign the value of 10 to all model cells.
5. Select *File* | *Leave Editor* or click the leave editor button .

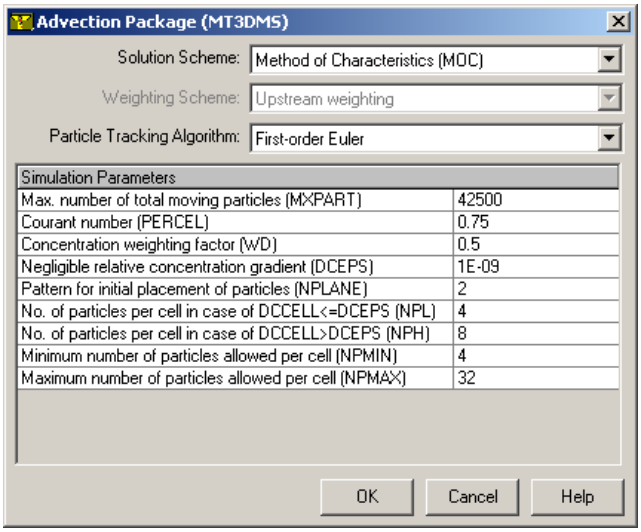

Advection Package (MT3DMS)
Solution Scheme:
Method of Characteristics (MOC)
Weighting Scheme:
Upstream weighting
Particle Tracking Algorithm:
First-order Euler
Simulation Parameters
Max. number of total moving particles (MXPART) 42500
Courant number (PERCEL) 0.75
Concentration weighting factor (WD) 0.5
Negligible relative concentration gradient (DCEPS) 1E-09
Pattern for initial placement of particles (NPLANE) 2
No. of particles per cell in case of DCCELL<=DCEPS (NPL) 4
No. of particles per cell in case of DCCELL>DCEPS (NPH) 8
Minimum number of particles allowed per cell (NPMIN) 4
Maximum number of particles allowed per cell (NPMAX) 32
OK
Cancel
Help

Fig. 4.20. The Advection Package (MT3DMS) dialog box

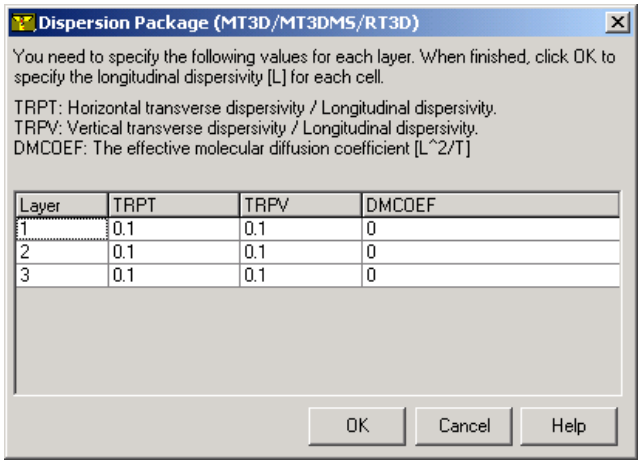


Fig. 4.21. The Dispersion Package (MT3D/MT3DMS/RT3D) dialog box

► To assign the chemical reaction parameters

1. Select *Models* | *MT3DMS* | *Chemical Reaction*.
   A Chemical Reaction Data (MT3DMS) dialog box appears.
2. In the Chemical Reaction Data (MT3DMS) dialog box, select the first species (which is only one species in this example), and click *Edit* to start the Data Editor.
3. Select *Value* | *Reset Matrix* (or press Ctrl+R).
   A Reset Matrix dialog box appears (Fig. 4.22). Set the *Type of Sorption* to "Linear equilibrium isotherm", and type 0.000125 for the distribution coefficient, then Click OK to assign the value to the first layer.
4. Turn on layer copy by clicking the layer copy button .
5. Move to the second layer and the third layer by pressing PgDn twice. The cell values of the first layer are copied to the second and third layers.
6. Select *File* | *Leave Editor* or click the leave editor button .
7. The Chemical Reaction Data (MT3DMS) dialog box appears again. Click *Close* to close this dialog box.

The last step before running the transport model is to specify the output times, at which the calculated concentration should be saved.

► To specify the output times

1. Select *Models* | *MT3DMS* | *Output Control*.
   The Output Control (MT3D Family) dialog box appears (Fig. 4.23). The options in this dialog box are grouped under three tabs - Output Terms, Output Times and Misc.
2. Click the Output Times tab, then click the header *Output Time* of the (empty) table.

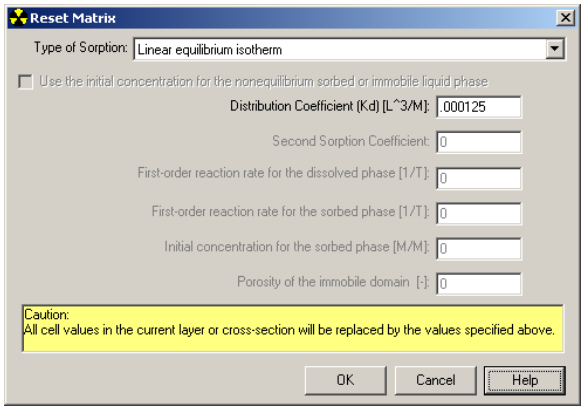

Reset Matrix
Type of Sorption:
Linear equilibrium isotherm
Use the initial concentration for the nonequilibrium sorbed or immobile liquid phase
Distribution Coefficient (Kd) [L^3/M]:
.000125
Second Sorption Coefficient:
0
First-order reaction rate for the dissolved phase [1/T]:
0
First-order reaction rate for the sorbed phase [1/T]:
0
Initial concentration for the sorbed phase [M/M]:
0
Porosity of the immobile domain [-]:
0
Caution:
All cell values in the current layer or cross-section will be replaced by the values specified above.
OK
Cancel
Help

Fig. 4.22. The Reset Matrix dialog box for chemical reaction data of MT3DMS

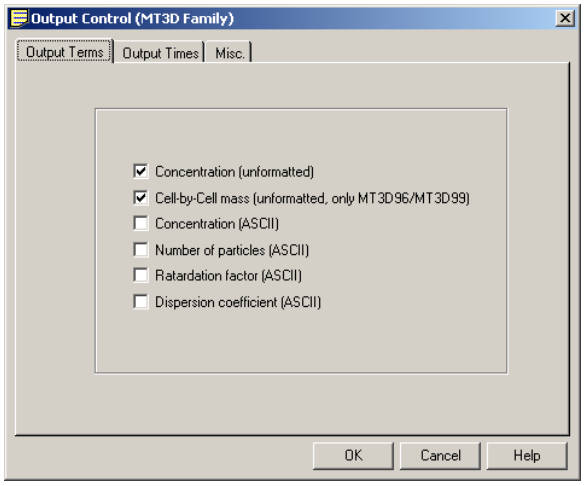


Fig. 4.23. The Output Control (MT3D Family) dialog box

An Output Times dialog box appears. Enter 3000000 to *Interval*. Click *OK* to accept the other default values.

3. Click OK to close the Output Control (MT3D Family) dialog box.

► To perform the transport simulation

1. Select *Models* | *MT3DMS* | *Run*.
   The Run MT3DMS dialog box appears (Fig. 4.24)
2. Click *OK* to start the transport computation. Prior to running MT3DMS, **PM** will use user-specified data to generate input files for MT3DMS as listed in the table of the Run MT3DMS dialog box. An input file will be generated, only if the corresponding Generate box is checked. You can click on the box to check

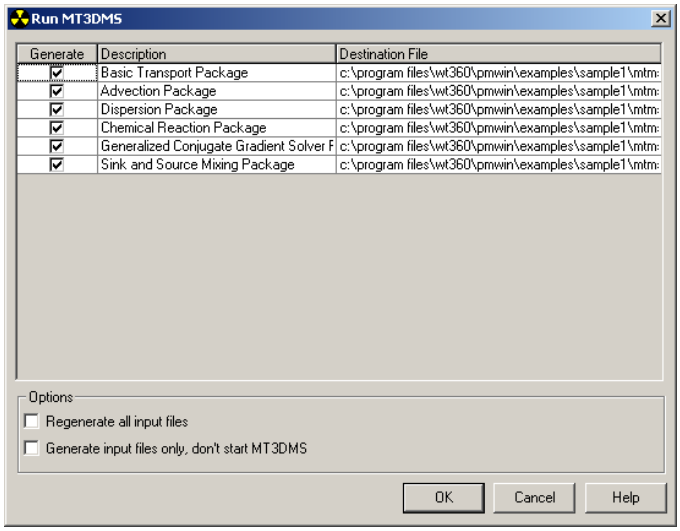


Fig. 4.24. The Run MT3DMS dialog box

or uncheck. Normally, we do not need to worry about these boxes since **PM** will take care of the settings.

► Check simulation results and produce output

During a transport simulation, MT3DMS saves a detailed run record *path**OUTPUT.MTM*, where *path* is the folder in which the model data is saved. In addition, MT3DMS saves the simulation results in various files. The output options are controlled by selecting *Models* | *MT3DMS* | *Output Control*.

To check the quality of the simulation results, MT3DMS calculates a mass budget at the end of each transport step and accumulated to provide summarized information on the total mass into or out of the groundwater flow system. The discrepancy between the in- and outflows of mass serves as an indicator of the accuracy of the simulation results. It is highly recommended to check the record file or at least take a glance at it.

Follow the steps below to generate contour maps of the calculated concentration values at the end of the simulation.

► To generate contour maps of the calculated concentration values

1. Select *Tools* | *2D Visualization*.
   A Result Selection dialog box appears.
2. Select the MT3DMS tab in the Result Selection dialog box.
3. Click *OK* to accept the default result type *Solute Concentration* and species 1.
   PM displays the model grid, sets the *Simulation Time* (on the toolbar) to the beginning of the simulation, and automatically loads the results pertained to the

Simulation Time. Contours are not visible at this stage, since the initial concentration values are zero over the entire model domain.

4. Click the *Simulation Time* drop-down list and set the simulation time to 9.467E+07 (the end of the simulation). By default, **PM** sets 10 contour levels ranging from the minimum to the maximum concentration values of the selected simulation time (Fig. 4.25). One can customize the contour levels and the appearance of the contours by using the Environment Options dialog box. Refer to Section 2.9.2 for details about this dialog box.
5. To save or print the graphics, select *File* | *Save Plot As* or *File* | *Print Plot*.
6. Select *File* | *Leave Editor* or click the leave editor button .

Follow the steps below to generate the concentration-time series curves at the observation boreholes.

► To generate the concentration-time series curves at the observation boreholes

1. Select *Models* | *MT3DMS* | *View* | *Concentration-Time Curves*.
   A Species dialog box appears.
2. In the Species dialog box, select the first species and click OK.
   PM displays the Time Series Curves (Concentration) dialog box (Fig. 4.26.) This dialog box has two tabs. The Data tab displays the calculated and measurement data (if any). The Chart tab displays the time-series curves. Refer to Section 2.6.1.20 for details about these tabs.
3. Click the Chart tab to display the curves (Fig. 4.27).

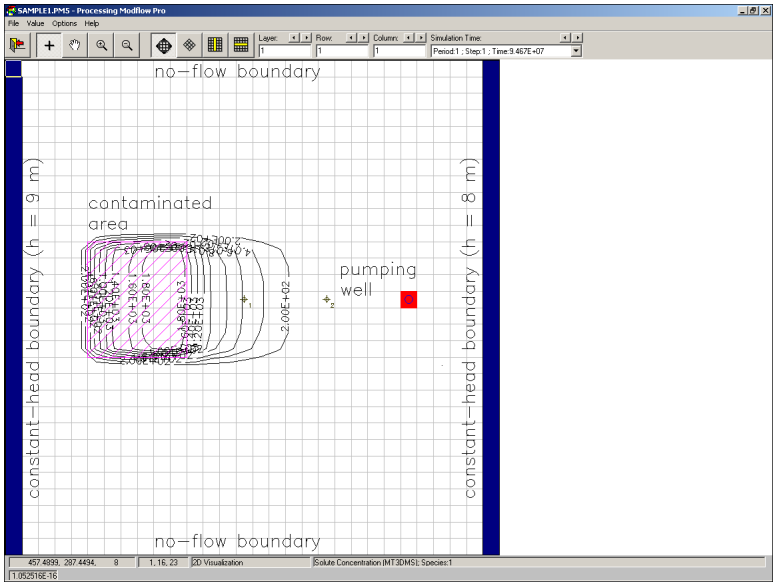


Fig. 4.25. Contours of the concentration values at the end of the simulation

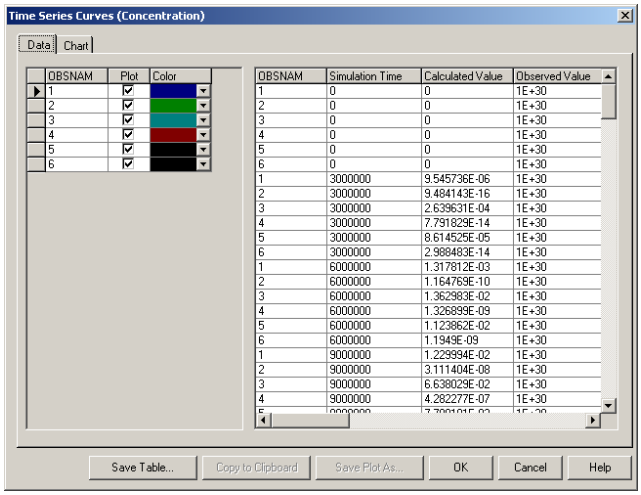


Fig. 4.26. The Time Series Curves (Concentration) dialog box

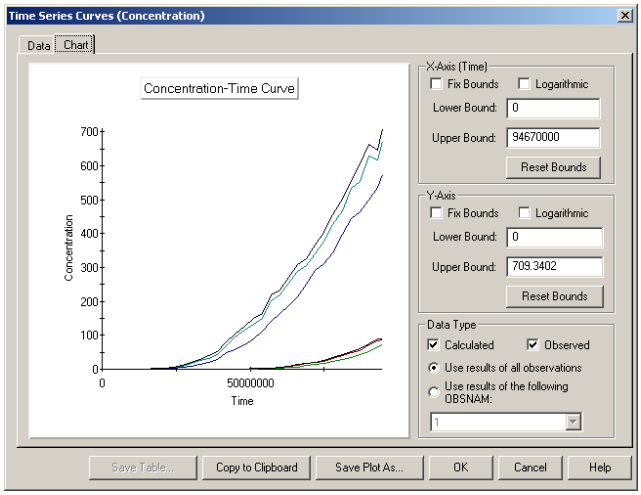


Fig. 4.27. The Chart tab of the Time Series Curves (Concentration) dialog box

4. Use the button *Save Plot As* to save the chart to a file or use *Copy to Clipboard* to copy the chart to the Windows Clipboard. An image in the clipboard can be pasted into most word- or graphics-processing software by using Ctrl+V.
5. Click OK to close the Time Series Curves (Concentration) dialog box.

4.1.3.2 Perform Transport Simulation with MOC3D

In MOC3D, transport may be simulated within a subgrid, which is a window within the primary model grid used to simulate flow. Within the subgrid, the row and column

spacing must be uniform, but the thickness can vary from cell to cell and layer to layer. However, the range in thickness values (or product of thickness and effective porosity) should be as small as possible.

The initial concentration must be specified throughout the subgrid within which solute transport occurs. MOC3D assumes that the concentration outside of the subgrid is the same within each layer; so only one value is specified for each layer within and adjacent to the subgrid. The use of constant-concentration boundary condition has not been implemented in MOC3D.

► To set the initial concentration

1. Select *Models* | *MOC3D* | *Initial Concentration*.
   For the current example, we accept the default value 0 for all cells.
2. Select *File* | *Leave Editor* or click the leave editor button .

► To define the transport subgrid and the concentration outside of the subgrid

1. Select *Models* | *MOC3D* | *Subgrid*.
   The Subgrid for Transport (MOC3D) dialog box appears (Fig. 4.28). The options in the dialog box are grouped under two tabs - Subgrid and C' Outside of Subgrid. The default size of the subgrid is the same as the model grid used to simulate flow. The default initial concentration outside of the subgrid is zero.
2. Click OK to accept the default values and close the dialog box.

► To assign the input rate of contaminants

1. Select *Models* | *MOC3D* | *Sink/Source Concentration* | *Recharge*.
2. Assign 12500 [$\mu g/m^3$] to the cells within the contaminated area.
   This value is the concentration associated with the recharge flux. Since the recharge rate is 8×10^{-9} [$m^3/m^2/s$] and the dissolution rate is 1×10^{-4} [$\mu g/s/m^2$], the concentration associated with the recharge flux is $1 \times 10^{-4}/8 \times 10^{-9} = 12500$ [$\mu g/m^3$].

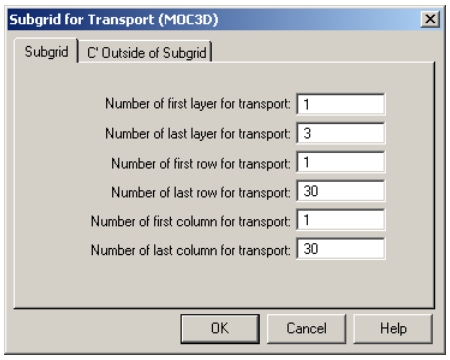


Fig. 4.28. The Subgrid for Transport (MOC3D) dialog box

3. Select *File* | *Leave Editor* or click the leave editor button .

► To assign the parameters for the advective transport

1. Select *Models* | *MOC3D* | *Advection* to display a Parameters for Advection Transport (MOC3D) dialog box.
2. Enter the values as shown in Fig. 4.29 into the dialog box.
3. Select Bilinear (X, Y directions) for the interpolation scheme for particle velocity. As given by Konikow and others [74] if transmissivity within a layer is homogeneous or smoothly varying, bilinear interpolation of velocity yields more realistic pathlines for a given discretization than does linear interpolation.
4. Click OK to close the dialog box.

► To assign the parameters for dispersion and chemical reaction

1. Select *Models* | *MOC3D* | *Chemical Reaction* to display a Dispersion / Chemical Reaction (MOC3D) dialog box. Check Simulate Dispersion and enter the values as shown in Fig. 4.30. The retardation factor R = 2 is calculated as follows:

$$R = 1 + \frac{\rho_b}{n_e} \cdot K_d = 1 + \frac{2000}{0.25} \cdot 0.000125 = 2 \tag{4.3}$$

   Note that the parameters for dispersion and chemical reaction are the same for each layer.
2. Click OK to close the dialog box.

► To set Strong/Weak Flag

1. Select *Models* | *MOC3D* | *Strong/Weak Flag*.
2. Move the grid cursor to the cell [1, 15, 25].

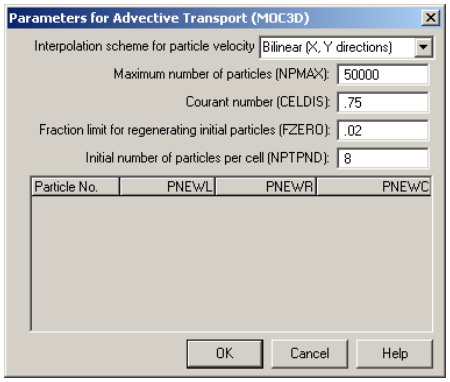


Fig. 4.29. The Parameters for Advective Transport (MOC3D) dialog box

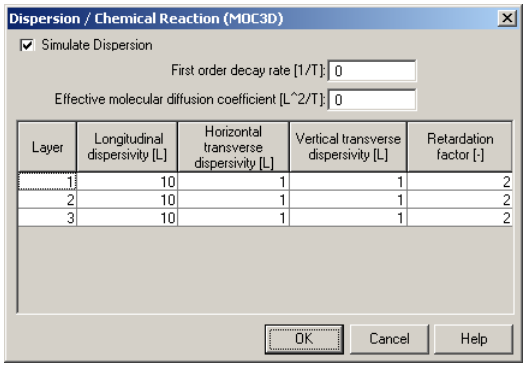


Fig. 4.30. The Dispersion / Chemical Reaction (MOC3D) dialog box

3. Press the right mouse button once to open a Cell Value dialog box, type 1 into the dialog box, then click OK. Note that a strong sink or source is indicated by the cell value of 1. When a fluid source is strong, new particles are added to replace old particles as they are advected out of that cell. Where a fluid sink is strong, particles are removed after they enter that cell.
4. Repeat steps 2 and 3 to assign the value 1 to the cells [2, 15, 25] and [3, 15, 25].
5. Select *File* | *Leave Editor* or click the leave editor button .

► To specify the output terms and times

1. Select *Models* | *MOC3D* | *Output Control*.
   An Output Control (MOC3D) dialog box appears. The options in the dialog box are grouped under five tabs - Concentration, Velocity, Particle Locations, Disp. Coeff. and Misc.
2. In the Concentration tab, select the option ”These data will be printed or saved every Nth particle moves”, and enter N = 20.
3. Click *OK* to accept all other default values and close the Output Control (MOC3D) dialog box (Fig. 4.31).

► To perform the transport simulation

1. Select *Models* | *MOC3D* | *Run*.
   The Run MOC3D dialog box appears (Fig. 4.32).
2. Click *OK* to start the transport computation.
   Prior to running MOC3D, **PM** uses user-specified data to generate input files for MOC3D as listed in the table of the Run MOC3D dialog box. An input file will be generated, only if the corresponding Generate box is checked. You can click on the box to check or uncheck. Normally, we do not need to worry about these boxes since **PM** will take care of the settings.

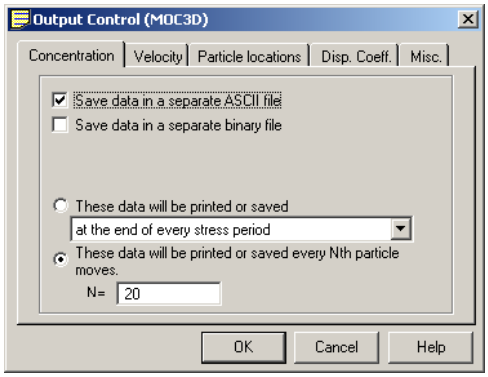


Fig. 4.31. The Output Control (MOC3D) dialog box

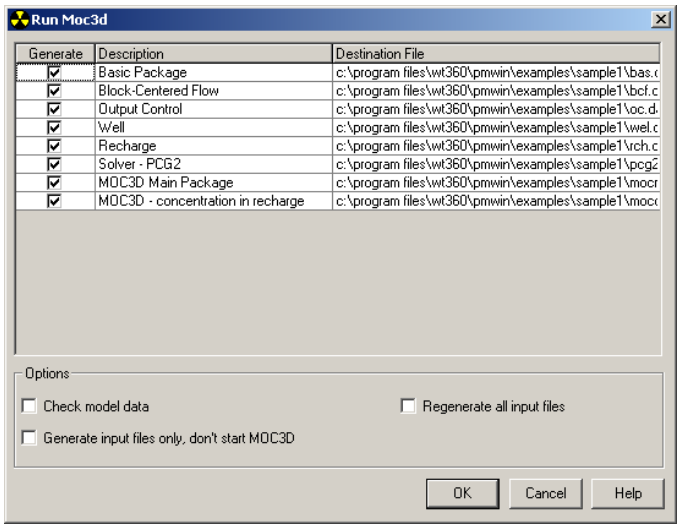


Fig. 4.32. The Run Moc3d dialog box

► Check simulation results and produce output

During a transport simulation, MOC3D writes a detailed run record to the file path\MOC3D.LST, where path is the folder in which your model data are saved. MOC3D saves the simulation results in various files, which can be controlled by selecting *Models* | *MOC3D* | *Output Control*.

To check the quality of the simulation results, MOC3D calculates mass balance and saves the results in the run record file. The mass in storage at any time is calculated from the concentrations at the nodes of the transport subgrid to provide summarized information on the total mass into or out of the groundwater flow system. The mass balance error will typically exhibit an oscillatory behavior over time, because of the nature of the method of characteristics and the finite-difference approxima-

tion. The oscillations reflect the fact that the mass balance calculation is itself just an approximation.

Follow the steps below to generate contour maps of the calculated concentration values at the end of the simulation.

► To generate contour maps of the calculated concentration values

1. Select *Tools* | *2D Visualization*.
   A Result Selection dialog box appears.
2. Select the MOC3D tab in the Result Selection dialog box.
3. Click *OK* to accept the default result type *Solute Concentration*.
   PM displays the model grid, sets the *Simulation Time* (on the toolbar) to the beginning of the simulation, and automatically loads the results pertained to the Simulation Time. Contours are not visible at this stage, since the initial concentration values are zero over the entire model domain.
4. Click the *Simulation Time* drop-down list and set the simulation time to 9.467E+07 (the end of the simulation). By default, **PM** sets 10 contour levels ranging from the minimum to the maximum concentration values of the selected simulation time (Fig. 4.33). One can customize the contour levels and the appearance of the contours by using the Environment Options dialog box. Refer to Section 2.9.2 for details about this dialog box.
5. To save or print the graphics, select *File* | *Save Plot As* or *File* | *Print Plot*.
6. Select *File* | *Leave Editor* or click the leave editor button .

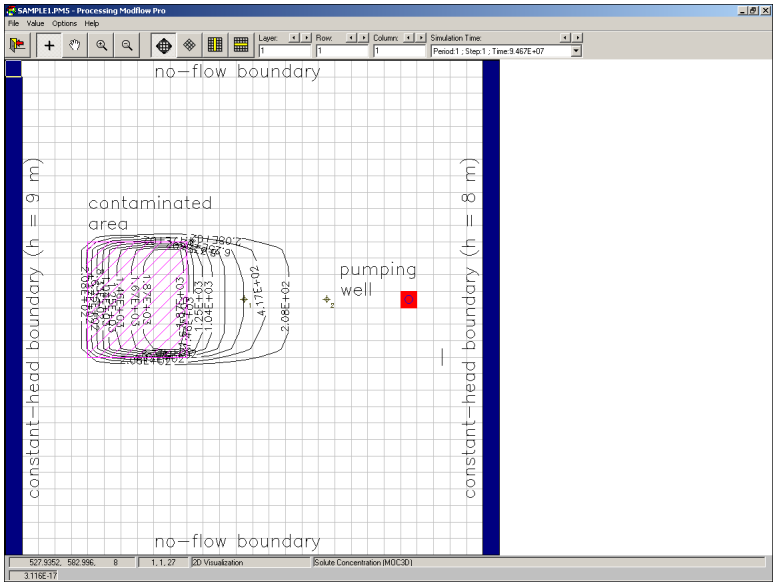


Fig. 4.33. Contours of the concentration values at the end of the simulation

Follow the steps below to generate the concentration-time series curves at the observation boreholes.

► **To generate the concentration-time series curves at the observation boreholes**

1. Select *Models* | *MOC3D* | *View* | *Concentration-Time Curves*.
   pmp displays the Time Series Curves (Concentration) dialog box (Fig. 4.34.) This dialog box has two tabs. The Data tab displays the calculated and measurement data (if any). The Chart tab displays the time-series curves. Refer to Section 2.6.1.20 for details about these tabs.
2. Click the Chart tab to display the curves (Fig. 4.35).
3. Use the button *Save Plot As* to save the chart to a file or use *Copy to Clipboard* to copy the chart to the Windows Clipboard. An image in the clipboard can be pasted into most word- or graphics-processing software by using Ctrl+V.
4. Click OK to close the Time Series Curves (Concentration) dialog box.

4.1.4 Parameter Estimation

The process of estimating unknown parameters is one of the most difficult and critical steps in the model application. The parameter estimation (often referred to as model calibration) of a flow model is accomplished by finding a set of parameters, hydrologic stresses, or boundary conditions so that the simulated values match the measurement values to a reasonable degree. Hill [62] gives methods and guidelines for model calibration using inverse modeling.

To demonstrate the use of the parameter estimation program PEST within **PM**, we assume that the hydraulic conductivity in the third layer is homogeneous but its

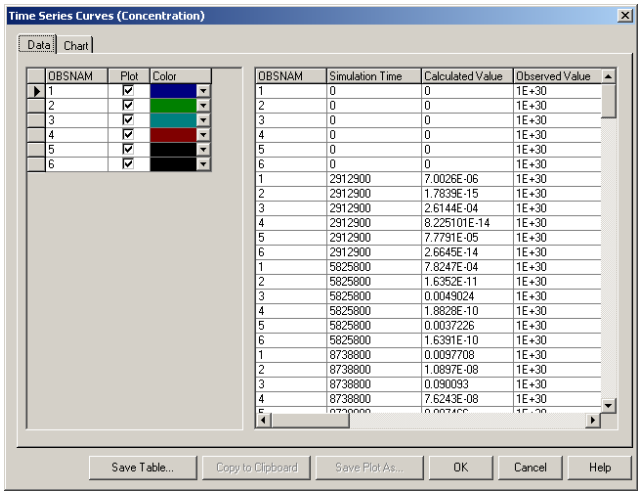


Fig. 4.34. The Time Series Curves (Concentration) dialog box

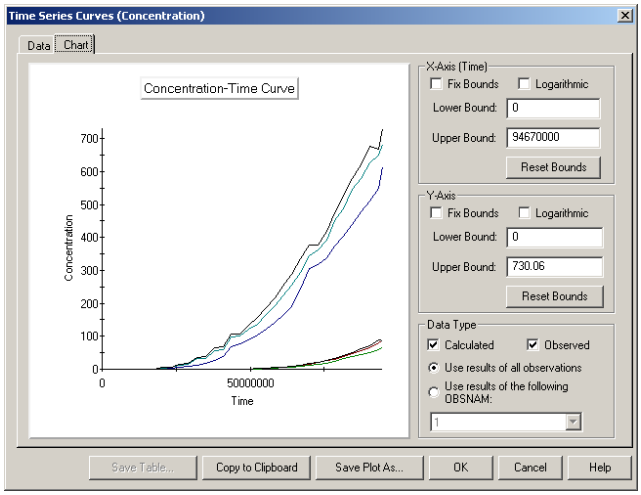


Fig. 4.35. The Chart tab of the Time Series Curves (Concentration) dialog box

value is unknown. We want to find out this value through a model calibration by using the measured hydraulic heads at the observation boreholes listed in Table 4.5. Three steps are required for the parameter estimation.

1. Define the region of each parameter.
   Parameter estimation requires a subdivision of the model domain into a small number of reasonable regions. A region is defined by using the Data Editor to assign a parameter number to the model cells.
2. Specify the coordinates of the observation boreholes and the measured hydraulic head values.
3. Specify the starting values, upper and lower bounds for each parameter.

► To define the region of horizontal hydraulic conductivity

1. Select *Parameters* | *Horizontal Hydraulic Conductivity*.
2. Click the button if the display mode is not Grid View.
3. Move to the third layer.
4. Select *Value* | *Reset Matrix* (or press Ctrl+R).
   A Reset Matrix dialog box appears.

Table 4.5 Measured hydraulic head values for parameter estimation

Borehole	X-Coordinate	Y-Coordinate	Layer	Observation Time	Hydraulic Head
h1	130	200	3	9.46728E+07	8.85
h2	200	400	3	9.46728E+07	8.74
h3	480	250	3	9.46728E+07	8.18
h4	460	450	3	9.46728E+07	8.26

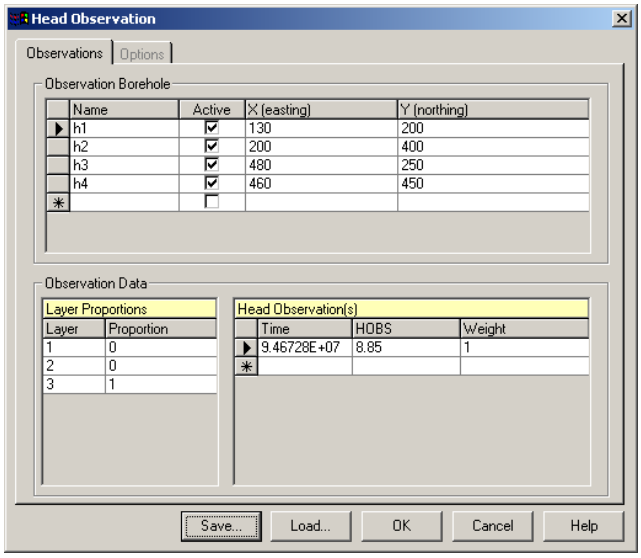


Fig. 4.36. The Head Observation dialog box

5. Enter 1 to the *Parameter Number* edit box, then click OK. The horizontal hydraulic conductivity of the third layer is set to the parameter #1.
6. Select *File* | *Leave Editor* or click the leave editor button .

► To specify the coordinates of the observation boreholes and measured values

1. Select *Head Observations* from the *MODFLOW*, *MODFLOW-2000 (Parameter Estimation)*, or *PEST (Parameter Estimation)* menu.
   The Head Observation dialog box appears (Fig. 4.36).
2. Enter the coordinates of the observation boreholes into the Observation Borehole table as shown in Fig. 4.36.
3. For all boreholes, set the proportion value of the third layer to 1 and other layers to 0. This means that all boreholes are screened in the third layer.
4. In the Head Observatiion(s) group, enter the observation time and hydraulic head of each borehole to *Time* and *HOBS*. Set the value for *Weight* to 1.
5. Click *OK* to close the dialog box.

4.1.4.1 Parameter Estimation with PEST

► To specify the starting values for each parameter

1. Select *Models* | *PEST* | *Parameter List*.
   The List of Parameters (PEST) dialog box (Fig. 4.37) appears. The options of the dialog box are grouped under five tabs - Parameters, Group Definitions, Prior Information, Control Data, and Options.

2. In the Parameters tab, enter values as shown in Fig. 4.37. PARVAL is the initial guess of the parameter. Minimum is the lower bound and Maximum is the upper bound of the parameter.
3. Click *OK* to close the dialog box.

► To perform Parameter Estimation with PEST

1. Select *Models* | *PEST* | *Run*.
   The Run PEST dialog box appears (Fig. 4.38).
2. Click *OK* to start PEST.
   Prior to running PEST, **PM** uses user-specified data to generate input files for PEST and MODFLOW as listed in the table of the Run PEST dialog box. An input file will be generated, only if the corresponding Generate box is checked. You can click on the box to check or uncheck. Normally, we do not need to worry about these boxes since **PM** will take care of the settings.

► Check the Parameter Estimation Results

Several result files are created through the parameter estimation process. During a parameter estimation process, PEST prints the estimated parameter values to the run record file PESTCTL.REC in the model folder and writes the estimated parameter values to the corresponding input files of MODFLOW (BCF.DAT, WEL.DAT,... , etc.). So, after a parameter process, the simulation results of MODFLOW are updated by using the most recently estimated parameter values. PEST does not modify the original model data. This provides a greater security to the model data since a parameter estimation process does not necessarily lead to a success. Follow the steps below if you want to operate on the estimated parameters.

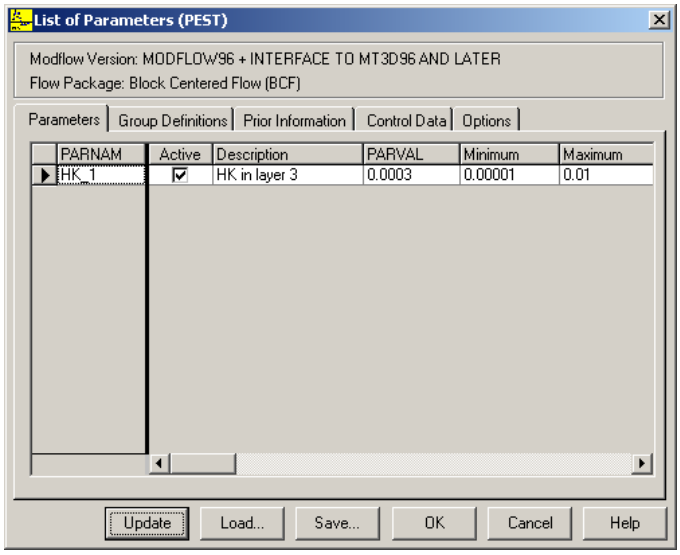


Fig. 4.37. The List of Parameters (PEST) dialog box

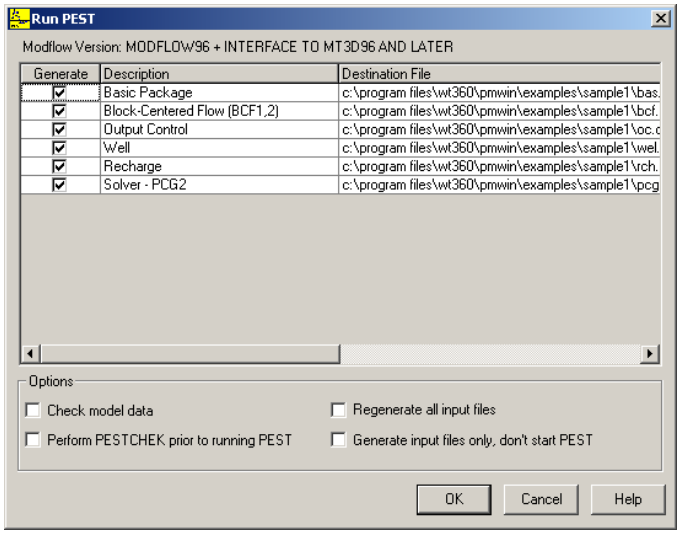


Fig. 4.38. The Run PEST dialog box

► To operate on the estimated parameters

1. Select *Models* | *PEST* | *Parameter List* to open the List of Parameters (PEST) dialog box.
2. Click the *Update* button to retrieve the estimated parameter values into the parameter list.
3. Click the *Options* tab and set the *Run Mode* to ”Perform Forward Model Run using PARVAL values given in the Parameters tab”.
4. Click *OK* to close the List of Parameters (PEST) dialog box.
5. Select *Models* | *PEST* | *Run* to run PEST in the forward model run mode.

Alternatively, you can create a new model with the estimated parameters by using the Convert Models dialog box (see Section 2.3.3 for details).

You can create a scatter diagram to present the parameter estimation result. The observed head values are plotted on one axis against the corresponding calculated values on the other. If there is an exact agreement between measurement and simulation, all points lie on a 45° line. The narrower the area of scatter around this line, the better is the match.

► To create a scatter diagram for head values

1. Select *Models* | *PEST* | *View* | *Head Scatter Diagram*.
   The Scatter Diagram (Hydraulic Head) dialog box appears (Fig. 4.39). This dialog box has two tabs. The Data tab displays the calculated and observed values. The Chart tab displays the scatter diagram. Refer to Section 2.6.1.20 for details about these tabs.
2. Click the Chart tab to display the scatter diagram (Fig. 4.40).

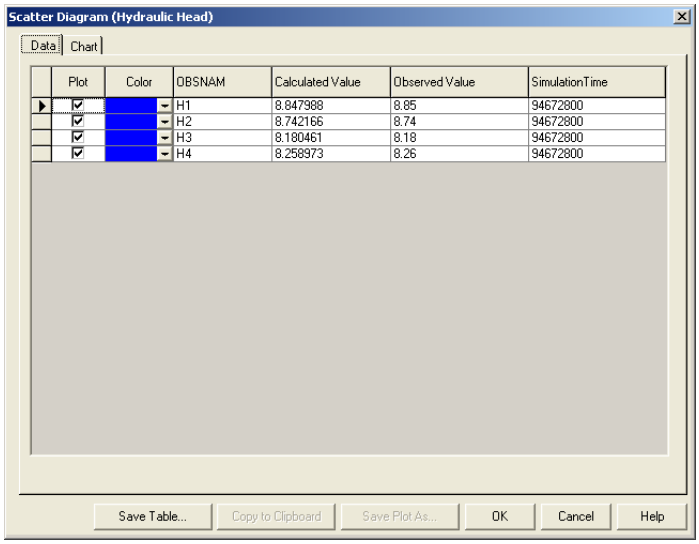


Fig. 4.39. The Scatter Diagram dialog box

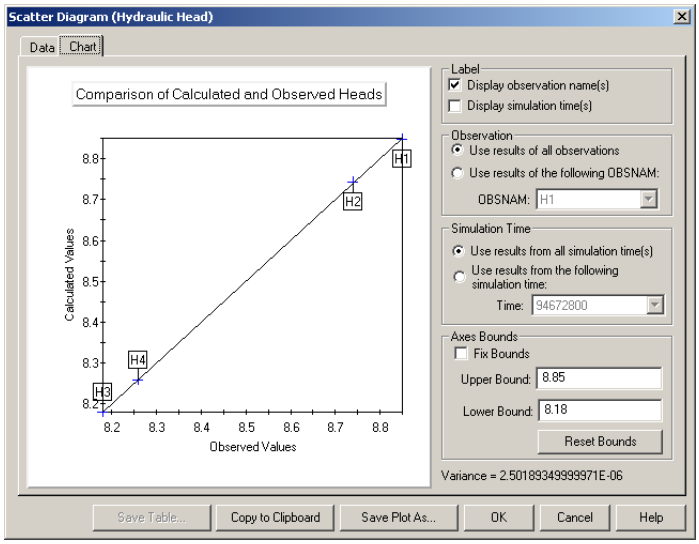


Fig. 4.40. The Chart tab of the Scatter Diagram dialog box

3. Use the button *Save Plot As* to save the chart to a file or use *Copy to Clipboard* to copy the chart to the Windows Clipboard. An image in the clipboard can be pasted into most word- or graphics-processing software by using Ctrl+V.
4. Click *OK* to close the Scatter Diagram (Hydraulic Head) dialog box

4.1.5 Animation

You already learned how to use the 2D Visualization tool to create and print contour maps of calculated head and concentration values. The saved or printed images are static and ideal for paper-based reports or slide-based presentations. In many cases, however, these static images cannot ideally illustrate the motion of concentration plumes or temporal variation of hydraulic heads or drawdowns. **PM** provides an animation technique to display a sequence of the saved images in rapid succession. Although the animation process requires relatively large amount of computer resources to read, process and display the data, the effect of a motion picture is often very helpful.

The 2D Visualization tool is used to create animation sequences. The following steps show how to use the Environment Options and Animation dialog boxes to create an animation sequence for displaying the motion of the concentration plume in the third layer.

► To create an animation sequence

1. Select *Tools* | *2D Visualization*.
2. Select the MT3DMS tab in the Result Selection dialog box.
3. Click *OK* to accept the default result type *Solute Concentration* and species 1. **PM** displays the model grid, sets the *Simulation Time* (on the toolbar) to the beginning of the simulation, and automatically loads the results pertained to the Simulation Time.
4. Click the *Simulation Time* drop-down list and set the simulation time to 9.467E+07 (the end of the simulation). By default, **PM** sets 10 contour levels ranging from the minimum to the maximum concentration values of the selected simulation time (Fig. 4.25). One can customize the contour levels and the appearance of the contours by using the Environment Options dialog box.
5. Click the button if the display mode is not Grid View.
6. Move to the third layer.
7. Select *Options* | *Environment*.
8. Click the *Contours* tab, clear *Display contour lines*, and check *Visible* and *Fill Colors*.
9. Click the table header *Level*.
   A Contour Levels dialog box appears. Set the value for *Minimum* to 100, *Maximum* to 1600 and *Interval* to 100. When finished, click *OK* to close the dialog box.
10. Click the table header *Fill*.
    A Color Spectrum dialog box appears. Set an appropriate color range by clicking the *Minimum color* and *Maximum color* buttons. When finished, click *OK* to close the dialog box.
11. Click *OK* to close the Environment Options dialog box.
12. Select *File* | *Animation*. The Animation dialog box appears (Fig. 4.41).

13. Click the button to display a Save File dialog box.
14. Select an existing file or specify a new base file name (without extension) in the or specify a file name in Save File dialog box, then click *Open*.
15. In the Animation dialog box, click *OK* to start the animation.
    PM will create a frame (image) for each time point at which the simulation results (here: concentration) are saved. Each frame is saved in filename.nnn, where filename is the base file name specified in previous step and nnn is the serial number of the frame. Note that if you have complex DXF-base maps, the process will be slowed down considerably. When all frames are created, **PM** will repeat the animation indefinitely until the *Esc* key is pressed.

Once a sequence is created, you can playback the animation at a later time by repeating steps 8 to 11 with the *Create New Frames* box cleared in step 10.

Note. Since the number and the size of the image files can be very large, make sure that there is enough free space on your hard disk. To reduce the file size, you can change the size of the **PM** window before creating the frames. You may also wish to turn off the display of the model grid in the Environment Options dialog box so that you don't have the grid cluttering the animation.

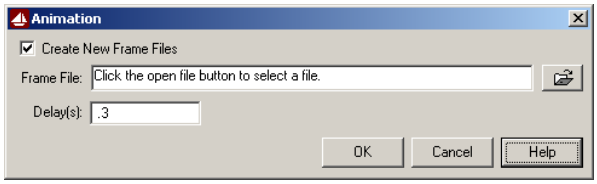


Fig. 4.41. The Animation dialog box

4.2 Unconfined Aquifer System with Recharge

Folder: *pmdir*\examples\tutorials\tutorial2

4.2.1 Overview of the Hypothetical Problem

The model assumes a simple scenario, which is designed to demonstrate the basic features of PMWIN and MODFLOW. An unconfined aquifer (Fig. 4.42) is a coarse grained sand with a measured isotropic hydraulic conductivity of 160 m/day, the specific yield has been assessed as 0.06. Recharge to the aquifer only occurs throughout the 4 month wet season at a rate of $7.5 \times 10^{-4} m/day$, outside the wet season there is no recharge to the aquifer. The elevations of the aquifer top and bottom are 25 m and 0 m, respectively. The area of interest is 10000 m long and 6000 m wide and is bounded by "no flow" zones to the east and west. There is also a volcanic mountain in the southeast corner of the model area. To the north an area of constant hydraulic head existed with a value of 15 m. The southern boundary is a specified flux boundary with an inflow rate of 0.0672 m^3/day per meter. A total of nine wells in the area are pumped at 45 l/s (3888 m^3/d) each during the 8-month dry season to supply water for irrigation and domestic purposes.

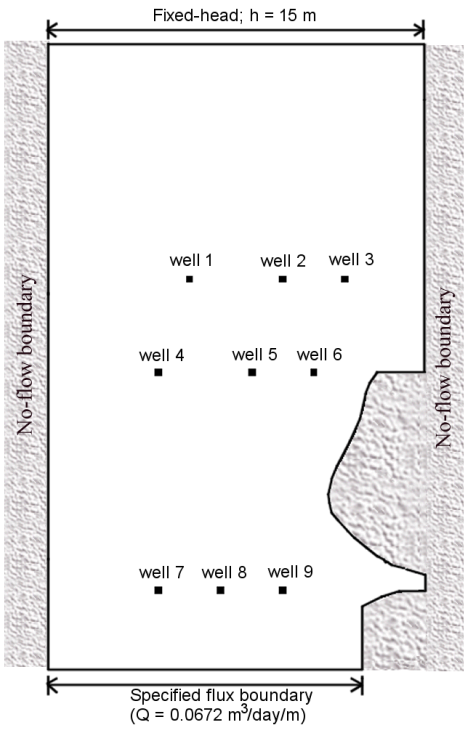


Fig. 4.42. Configuration of the hypothetical model

The task is to assess the water levels in the aquifer under the following conditions:

1. Steady-state, with the mean recharge rate = $2.5 \times 10^{-4} m/day$, no pumping;
2. After 8 months pumping during the dry season; and
3. The water levels by the end of the followed 4-month wet season.

4.2.2 Steady-state Flow Simulation

Seven main steps need to be done in this tutorial:

1. Create a new model,
2. Generate the model grid,
3. Refine the model grid,
4. Assign the model data,
5. Perform steady-state flow simulation,
6. Extract and view results,
7. Produce output from the steady-state simulation

4.2.2.1 Step1: Create a New Model

The first step in running a flow simulation is to create a new model.

► To create a new model

1. Select *File* | *New Model*. A New Model dialog box appears. Select a folder for saving the model data, such as C:\Models\tutorial2, and type the file name TUTORIAL2 as the model name. A model must always have the file extension .PM5. All file names valid under MS-Windows with up to 120 characters can be used. It is a good idea to save every model in a separate folder, where the model and its output data will be kept. This will also allow **PM** to run several models simultaneously (multitasking).
2. Click *OK*.
   PM takes a few seconds to create the new model. The name of the new model name is shown in the title bar.

4.2.2.2 Step2: Generate the Model Grid

► To generate the model grid

1. Select *Grid* | *Mesh Size*.
   A Model Grid and Coordinate System dialog box appears.
2. Enter the values as shown in Fig. 4.43 to the dialog box.
3. Click *OK* to close the dialog box.

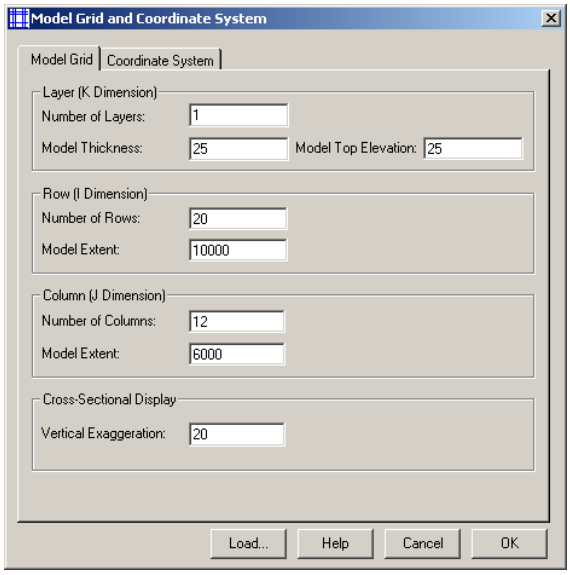


Fig. 4.43. The Model Grid and Coordinate System dialog box

You are now in the Grid Editor of **PM**. To help visualize the model site we can overlay a DXF file as a site map, which gives us the locations of the boundaries and the pumping wells.

► **To load a map**

1. Select *Options* | *Map* to open the Map Options dialog box.
2. Right-click on the first DXF File field to bring up the Map Files dialog box and then select the file BASEMAP.DXF from the folder \examples\tutorials\tutorial2\.
3. Check the box at the front of the DXF File field. The map will be displayed only if the box is checked.
4. Click *OK* to close the Map Options dialog box.
5. Select *File* | *Leave Editor* or click the leave editor button .

4.2.2.3 Step 3: Refine the Model Grid

It is a good practice to use a smaller grid in areas where the hydraulic gradient is expected to be large, which are normally located around the wells. In **PM**, grid refinement takes place within the Grid Editor and it is quite easy to add additional rows and columns to an existing model grid. This is done by using a combination of holding down the CTRL key and using the arrow keys as follows:

– CTRL + Up arrow - add a row
– CTRL + Down arrow - remove an added row
– CTRL + Right arrow - add a column

– CTRL + Left arrow - remove an added column.

It is also possible to specify the row and column spacing of individual cells by clicking the right mouse button within the cell of interest, however we will not be doing that in this exercise.

► **To refine the model grid around the pumping wells**

1. Select *Grid* | *Mesh Size* to open the Grid Editor.
2. Zoom in around Well 1 by clicking on the button and then dragging a box around the area of Well 1.
3. Click the button and click on the cell containing Well 1.
4. Divide this column into three by adding two additional columns with
   CTRL + Right arrow followed by
   CTRL + Right arrow
5. Divide the row also into three by adding two additional rows with
   CTRL + Up arrow followed by
   CTRL + Up arrow
   You should see dashed lines where the new rows and columns will be placed.
6. Zoom out by pressing the button. You will notice that the rows and columns added extend throughout the model domain and form part of the fine discretization around some of the other wells.
7. Repeat the above refinement around Well 2 to Well 9, remember some of the discretization has already been done when you added rows and columns around Well 1.
8. At this stage the model cells change from a size of 167 m to 500 m abruptly. In order to have a more gradual size change we need to half the size of the following rows and columns (again using the CTRL key and the arrow keys).
   Columns 3 and 11
   Rows 7, 9, 10, 12, 17, and 19.
   Upon completion of the refinement your grid should look like that in Fig. 4.44.
9. Select *File* | *Leave Editor* or click the leave editor button .

4.2.2.4 Step 4: Assign Model Data

The Data Editor is accessed each time when spatial data (such as recharge, hydraulic conductivity etc.) need to be input to the model. The format and commands of the Data Editor are the same for each parameter and once you become familiar with the commands and menus it is very easy to enter and change the model data. The values of the particular data being edited or entered and the selected cell are displayed in the status bar on the bottom of the screen.

The model data for task #1 (steady-state water level, with recharge, no pumping) includes layer properties, model boundaries, aquifer geometry, aquifer parameters, initial conditions, time parameters, and recharge rates.

► **To define the layer properties**

1. Select *Grid* | *Layer Property*.
   A Layer Options dialog box appears.
2. In the Layer Options dialog box, click on Type and select Unconfined, it is okay to browse through the rest of this dialog box, but leave all the values as the default ones.
3. Click *OK* to close the Layer Options dialog box.

► **To define the model boundaries**

1. *Select Grid* | *Cell Status* | *IBOUND (Modflow)*.
   MODFLOW uses a cell status array called the IBOUND array to determine if a particular cell is active, inactive (no flow) or a constant head cell. Cell values within IBOUND are as follows:
   active = 1 (or other positive integers)
   inactive = 0
   fixed-head = -1 (or other negative integers)
   These values are assigned to cells as required in the Data Editor. By default and

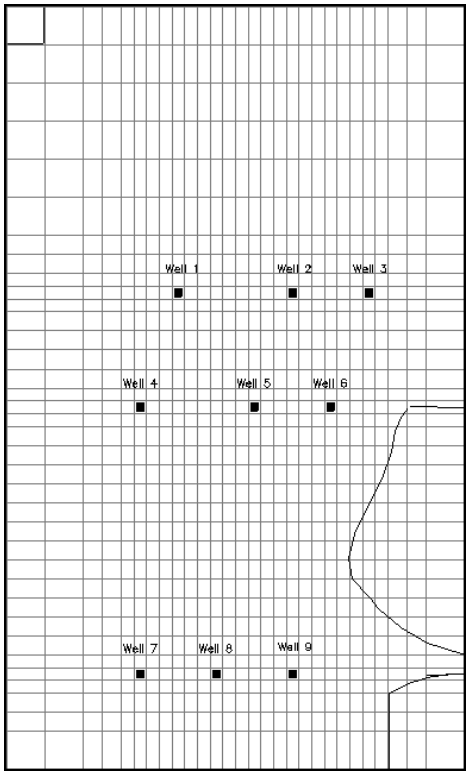


Fig. 4.44. Model grid after the refinement

convention the area outside the model domain is deemed to be a ”no flow zone” and as such it is not necessary to set this area to inactive.

2. Click the button if the display mode is not Grid View.
3. Make sure the cell selected is [1, 1, 1], and press *Enter* or right-click to open the Cell Value dialog box. Since this is going to be a constant head boundary enter -1, and click *OK* to exit the dialog box. The cell should now have a blue color signifying that it has been set as constant head.
   To save doing this for the remaining constant head cells it is possible to copy the value (in this case -1) to any other cell.
4. Click on the Duplication button, duplication is activated if the button is depressed.
5. Simply left-click in any cell that you want to specify as a constant head cell. If you make a mistake, turn off Duplication by clicking the duplication button and right-click in the cell where you have made a mistake and replace it with the desired value.
6. Complete specification of the entire North boundary as constant head cells. We will assign a head value to these cells a little later.

The outer grid boundaries are assigned as No Flow by default. However, the mountain area in the south corner of the domain, which is impervious and still falls inside the model grid, needs to be explicitly assigned as No Flow (i.e. IBOUND=0).

► To specify the no-flow zone

1. Ensure Duplication is off and then click in a cell within the No Flow zone.
2. Press *Enter* or Right-click the cell to open the Cell Value dialog box.
3. Enter 0 as the value for IBOUND and click *OK* to exit the dialog box.
   You will notice that the cell is now gray in color.
4. Either repeat the above 3 steps for the remaining no flow cells or turn on the Duplication and copy the value of IBOUND = 0 to the other cells. In some cases you will notice that the boundary cuts through part of a cell. In these cases you need to make a judgment as to whether the cell should remain active (IBOUND=1) or be specified as inactive (IBOUND=0). Generally, you should choose the option, which applies to more than 50% of the cell area. If all the steps were completed correctly, the grid should now look similar to that in Fig. 4.45
5. Select *File* | *Leave Editor* or click the leave editor button.

The next step in the modeling process is to specify the top and bottom elevations of the model layer.

► To specify the elevation of the top of the model layer

1. Select *Grid* | *Top of Layers (TOP)*.
2. Since the aquifer top elevation is uniform throughout the model it is possible to set a single value to the entire grid by selecting *Value* | *Reset Matrix*.
3. Enter 25 in the Reset Matrix dialog box and click *OK* to exit.

4. Select *File* | *Leave Editor* or click the leave editor button .

Repeat the above process to set the elevation of the base of the aquifer to 0 m. Although the default value in this model is zero, we still have to enter the editor to let the model know that the parameter has been specified.

► To specify the horizontal hydraulic conductivity

1. Select *Parameters* | *Horizontal Hydraulic Conductivity*.
2. Since the horizontal hydraulic conductivity is uniform throughout the model it is possible to set a single value to the entire grid by selecting *Value* | *Reset Matrix*.
3. Enter 160 in the Reset Matrix dialog box and click *OK* to exit.
4. Select *File* | *Leave Editor* or click the leave editor button .

MODFLOW requires initial hydraulic head conditions to enable it to perform the flow simulation. The hydraulic head values of the constant head cells are important as these do not change throughout the simulation. The values in the other cells serve as initial guesses for the iterative solvers. In a transient simulation, the hydraulic heads at the start of the simulation are the basis for determining the resulting head

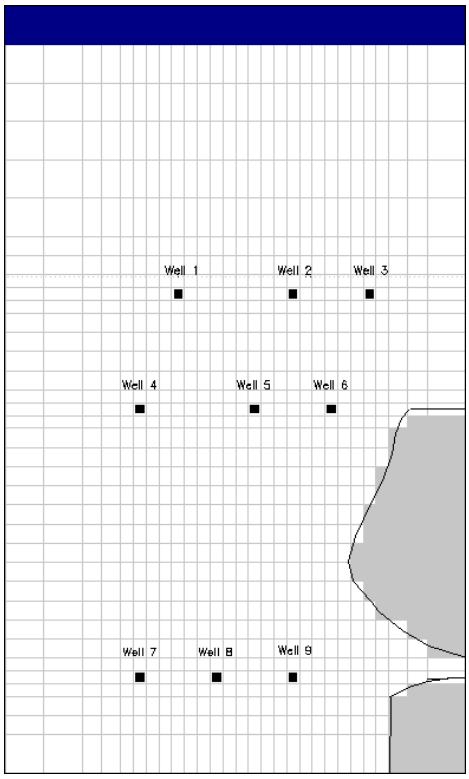


Fig. 4.45. Model Boundaries

distribution after the aquifer is subject to some time-dependent stresses. It is usual to perform a steady state flow simulation first and use the resulting head distribution as the basis for the transient simulations, which is what we shall do in this case.

► To set the initial hydraulic heads

1. Select *Parameters* | *Initial & Prescribed Hydraulic Heads*.
2. First set the entire grid to a uniform value by selecting *Value* | *Reset Matrix*.
3. Enter 16 in the Reset Matrix dialog box and click *OK* to exit.
4. Now set hydraulic head of the northern constant head boundary to 15 meters by first selecting the top left cell [1, 1, 1] with the left mouse button and then assigning a value of 15 by pressing *Enter* or right-clicking, and entering 15 in the Cell Value dialog box.
5. Copy the value of 15 to the remainder of the northern boundary using the Duplication button and the left mouse button.
6. Select *File* | *Leave Editor* or click the leave editor button .

► To specify the time parameters

1. Select *Parameters* | *Time*.
2. In the Time Parameters dialog box, change the *Simulation Time Unit* to DAYS and check that *Steady State* is selected in the *Simulation Flow Type* box.
3. Click *OK* to leave the Time Parameters dialog box.

► To specify the recharge rate

1. Select *Models* | *MODFLOW* | *Recharge*.
2. Set the entire grid to a uniform value by selecting *Value* | *Reset Matrix*.
3. In the Reset Matrix dialog box enter,
   - Recharge Flux [LT^{-1}] = 0.00025 (this is the mean recharge rate of the two seasons).
   - Layer Indicator [IRCH] = 0.
   - Recharge Options: Recharge is applied to the highest active cell.
4. Click *OK* to exit the dialog box.
5. Select *File* | *Leave Editor* or click the leave editor button .

► To specify the boundary flux

1. Select *Models* | *MODFLOW* | *Well*.
   Since MODFLOW does not have a separate package for a specified flux boundary condition, we use the Well package to simulate this boundary condition.
2. Make sure the cell selected is [1, 36, 1]. Since the width of this cell is 500 m, the inflow rate through this cell is $500m \times 0.0672m^3/day/m = 33.6m^3/day$. Press *Enter* or right-click to open the Cell Value dialog box, enter 33.6, then click *OK* to exit the dialog box. A positive value means that water enters the system.
3. Specify the value 33.6 to the cell [1, 36, 2], the value 16.8 to the cells [1, 36, 3] and [1, 36, 4], and the value 11.2 to the rest of the South boundary.

4. Select *File* | *Leave Editor* or click the leave editor button .

4.2.2.5 Step 5: Perform steady-state flow simulation

You are just about ready to run the flow model. Quickly review the data that you have entered for each of the parameters by checking the values of various cells. Correct any data that does not look right, by redoing the appropriate sections above.

► To run the flow simulation

1. Select *Models* | *Modflow* | *Run*.
2. Click OK to accept the warning regarding the Effective Porosity.
3. Click OK in the Run Modflow dialog box to generate the required data files and to run MODFLOW, you will see a DOS window open and MODFLOW perform the iterations required to complete the flow simulation.
4. Press any key to exit the DOS Window.

4.2.2.6 Step 6: Extract and view results

It is now time to view the results of your efforts, but first it is necessary to understand how the Results Extractor operates. On occasions it is necessary to view some of the various sorts of output such as hydraulic heads and cell-by-cell flows generated by a MODFLOW simulation. This layer-wise data is accessed using 2D Visualization tool. It is quite a simple procedure to load and save any of the output generated by MODFLOW.

► To generate contour maps of the calculated heads

1. Select *Tools* | *2D Visualization* to display a Result Selection dialog box.
2. Click *OK* to select the default result type *Hydraulic Head*.
   PM displays the model grid and head contours. By default, **PM** sets 10 contour levels ranging from the minimum to the maximum value. You can customize the appearance of the contour lines by using the Environment Options dialog box.
3. Select *Options* | *Environment* to open the Environment Options dialog box to customize the appearance of the contours.
   Click the Contours tab and make sure the *Visible* box is checked. Click on the header *Level* of the table to change the contour minimum to 12.5, maximum to 19 and the contour interval to 0.5. It is also possible to change contour color if you desire. If *Fill Contours* is checked, the contours will be filled with the colors given in the *Fill* column of the table. Use the *Label Format* button to specify an appropriate format.
4. Click *OK* to close the Environment Options dialog box. Contours should now appear and if everything has gone well they will look similar to Fig. 4.46. Note. The display of the model grid is deactivated by using the Appearance tab of the Environment Options dialog box.

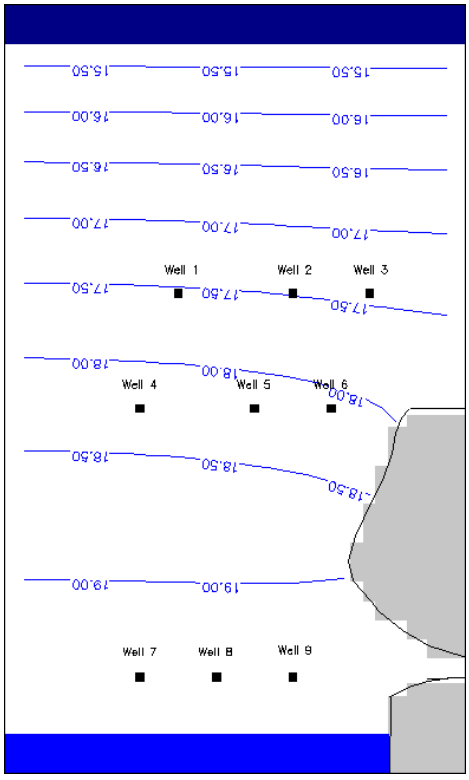


Fig. 4.46. Steady state head distribution

5. To save or print the graphics, select *File* | *Save Plot As* or *File* | *Print Plot*.
6. You may save the calculated head values in ASCII Matrix files by selecting *Value* | *Matrix* to open a Browse Matrix dialog box, and then clicking the *Save* button.
7. Select *File* | *Leave Editor* or click the leave editor button .

4.2.3 Transient Flow Simulation

It is now time to perform the transient simulations with the wet season recharge (120 days) and dry season pumping (240 days). The hydraulic heads resulting from the steady state simulation are used as the starting heads for the transient analysis.

► To set the steady state heads as the starting values for the simulation

1. Select *Parameters* | *Initial & Prescribed Hydraulic Heads* to start the Data Editor.
2. Select *Value* | *Import Results* to open an Import Results dialog box.
3. Click *OK* to import the hydraulic head (it is the default result type) from the first time step of the first stress period.

4. Select *File* | *Leave Editor* or click the leave editor button .

We now need to change from a steady state simulation to a transient simulation. In the transient simulation there are two stress periods, one of 240 days when pumping is occurring and no recharge and the other of 120 days when there is recharge only. It is possible to have different conditions for each stress period as will be demonstrated below.

► To change to a transient simulation

1. Select *Parameters* | *Time* to open the Time Parameters dialog box.
2. Change the model to transient by clicking on *Transient* in the *Simulation Flow Type* box.
3. Activate the second period by checking the *Active* box in the second row of the table.
4. Change the length of periods and numbers of time steps such that
   For period 1: Period Length = 240; Time Steps = 12
   For period 2: Period Length = 120; Time Steps = 6
5. Click *OK* to close the Time Parameters dialog box.

Now we need to set the pumping rate for each well during stress period 1.

► To set the pumping rate

1. Select *Models* | *MODFLOW* | *Well*.
2. The status bar displays Period 1 indicating that you are entering data for stress period 1.
3. At each of the wells (marked by a little shaded box on the DXF Map), left-click to select the cell and then right-click to set the pumping rate to -3888 m^3/d in the Cell Value dialog box. This pumping rate is equivalent to 45 l/s; the negative sign means that water is being extracted from the system. A recharge well would have a positive sign.
4. Click the Change Stress Period button to open a Temporal Data dialog box, this allows you to select and edit the data so that different values can apply during different Stress Periods.
5. In the Temporal Data dialog box, select Period 2 and click the *Edit Data* button. The status bar displays Period 2 indicating that you are entering data for stress period 2.
6. For each well in the system set the pumping rate to 0.
7. Select *File* | *Leave Editor* or click the leave editor button .

There are two recharge periods, namely the dry season when recharge is zero and the wet season when recharge is $7.5 \times 10^{-4} m/day$.

► To set the recharge rate

1. Select *Models* | *MODFLOW* | *Recharge*.

2. The status bar displays Period 1 indicating that you are entering data for stress period 1.
3. Set the entire grid to a uniform value for the first stress period by selecting *Value* | *Reset Matrix* to open a Reset Matrix dialog box.
4. In the Reset Matrix dialog box enter the following values then click OK to close the dialog box.
   - Recharge Flux [LT^{-1}] = 0.0
   - Layer Indicator [IRCH] = 0.
   - Recharge Options: Recharge is applied to the highest active cell.
5. Click the Change Stress Period button to open a Temporal Data dialog box, select Period 2, then click the *Edit Data* button.
   The status bar displays Period 2 indicating that you are entering data for stress period 2.
6. Use the above procedure to change the recharge flux for the entire grid to 0.00075 (the values for the layer indicator and recharge option remain the same).
7. Select *File* | *Leave Editor* or click the leave editor button .

Before running a transient simulation, it is necessary to specify storage terms, which account for the amount of water stored or released from aquifer matrix due to changes in hydraulic heads. For an unconfined layer, MODFLOW requires the storage term "specific yield".

► To specify the specific yield

1. Select *Parameters* | *Specific Yield*.
2. Select *Value* | *Reset Matrix* to set the entire grid to 0.06.
3. Select *File* | *Leave Editor* or click the leave editor button .

► To run the transient model

1. Select *Models* | *MODFLOW* | *Run*.
2. Click *OK* to accept the warning regarding the Effective Porosity.
3. Click *OK* in the Run Modflow dialog box to generate the required data files and to run MODFLOW, you will see a DOS window open and MODFLOW performs the iterations required to complete the flow simulation. By default, the simulation results at the end of each time step are saved. Refer to Section 2.6.1.18 (page 74) for more about Output Control.
4. Press any key to exit the DOS Window.

► To create head contours

Using the 2D Visualization, you can create contour plots for the water levels at the end of each time step. The water level at the end of the pumping period (dry season) corresponds to the heads in time step 12 of period 1 (Fig. 4.47a). The water level at the end of the recharge period (wet season) corresponds to the heads in time step 6 of

period 2 (Fig. 4.47b). Both figures use the contour interval of 0.5 m. The minimum and maximum contour levels are 12.5 m and 19 m respectively.

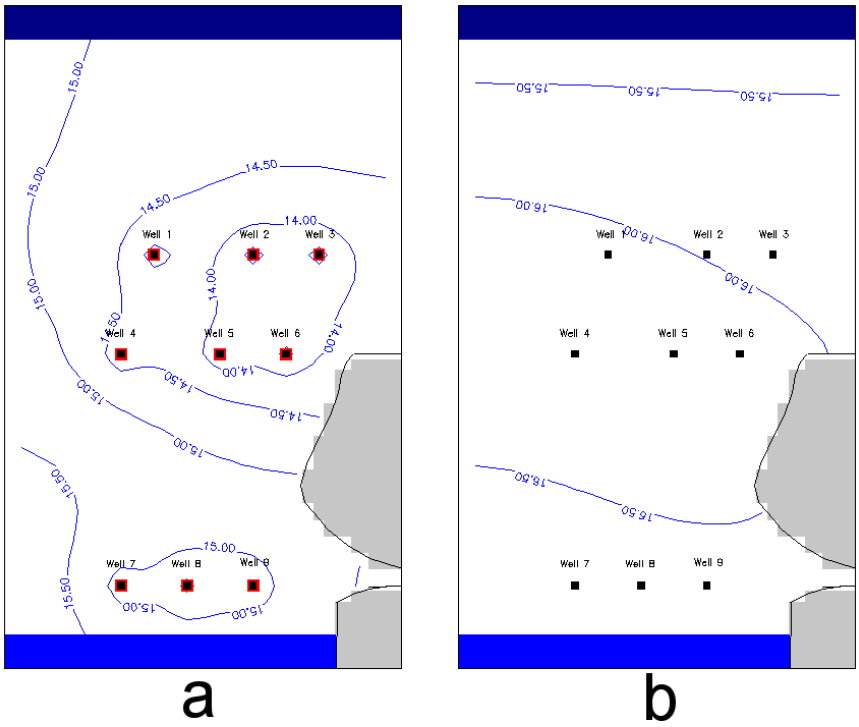


Fig. 4.47. (a) Head distribution after 240 days of pumping (period 1, time step 12) (b) Head distribution after 120 days of recharge (period 2, time step 6)

4.3 Aquifer System with River

Folder: *pmdir*\examples\tutorials\tutorial3

4.3.1 Overview of the Hypothetical Problem

A river flows through a valley (Fig. 4.48), which is bounded to the north and south by impermeable granite intrusions. The hydraulic heads at the upstream and downstream constant head boundaries are known (which are saved in a data file). The river forms part of a permeable unconfined aquifer system (horizontal hydraulic conductivity $HK = 5\ m/day$, vertical hydraulic conductivity $VK = 0.5m/day$, specific yield $S_y = 0.05$, effective porosity $n_e = 0.2$), which overlies a confined aquifer of a variable thickness ($HK = 2\ m/day$, $VK = 1\ m/day$, specific storage $S_s = 5 \times 10^{-5}$, $n_e = 0.25$). A silty layer ($thickness = 2\ m$, $KH = 0.5\ m/day$, $VK = 0.05\ m/day$, $n_e = 0.25$) separates the two aquifers. The elevations of the aquifer tops and bottoms are known (and saved in ASCII Matrix files). Three pumping wells pumping at $500m^3/day$ each abstracts water from the confined aquifer.

The river has the following properties:

- River stage = $19.4\ m$ on the upstream boundary.
- River stage = $17\ m$ on the downstream boundary.
- river width = $100\ m$.

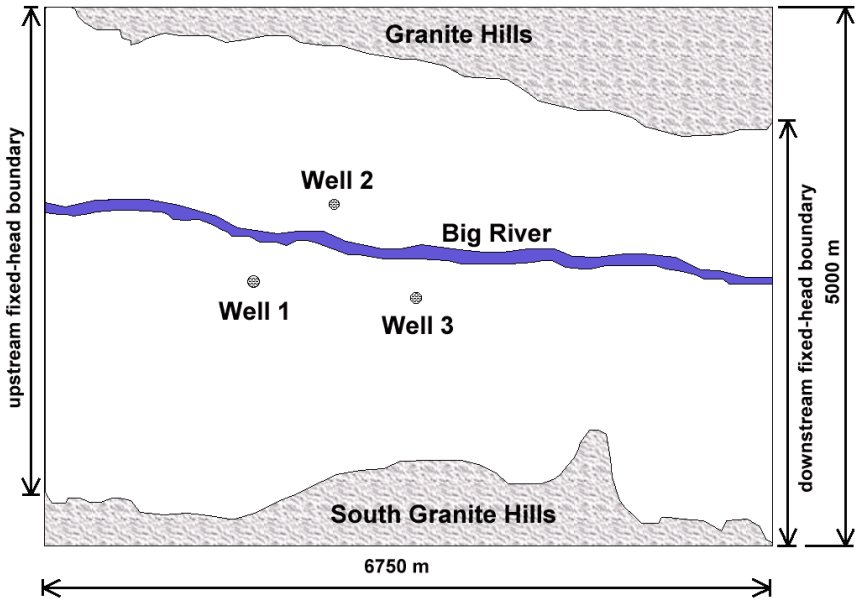


Fig. 4.48. Configuration of the hypothetical model

– riverbed hydraulic conductivity = 2 m/day.
– riverbed thickness = 1 m.
– Riverbed bottom elevation = 17.4 m on the upstream boundary.
– Riverbed bottom elevation = 15 m on the downstream boundary.

The task is to construct a 3-layer groundwater flow model of the area including the river and the pumping wells and to determine the capture zone of the wells. Seven main steps need to be done in this tutorial:

1. Create a new model,
2. Generate the model grid,
3. Refine the model grid,
4. Assign the model data,
5. Perform steady-state flow simulation,
6. Extract and view results,

4.3.1.1 Step 1: Create a New Model

The first step in running a flow simulation is to create a new model.

► To create a new model

1. Select *File* | *New Model*. A New Model dialog box appears. Select a folder for saving the model data, such as C:\Models\tutorial3, and type the file name TUTORIAL3 as the model name. A model must always have the file extension .PM5. All file names valid under MS-Windows with up to 120 characters can be used. It is a good idea to save every model in a separate folder, where the model and its output data will be kept. This will also allow **PM** to run several models simultaneously (multitasking).
2. Click *OK*.
   PM takes a few seconds to create the new model. The name of the new model name is shown in the title bar.

4.3.1.2 Step 2: Generate the Model Grid

► To generate the model grid

1. Select *Grid* | *Mesh Size*.
   A Model Grid and Coordinate System dialog box appears.
2. Enter the values as shown in Fig. 4.49 to the dialog box. The values for the *Model Thickness* and *Model Top Elevation* are not relevant at this stage, since we are going to import the elevations from disk files. We will generate a model grid of 3 layers. The unconfined aquifer is the layer 1 in the model. The silty layer and the confined aquifer are represented by layer 2 and layer 3, respectively.
3. Click *OK* to close the dialog box.

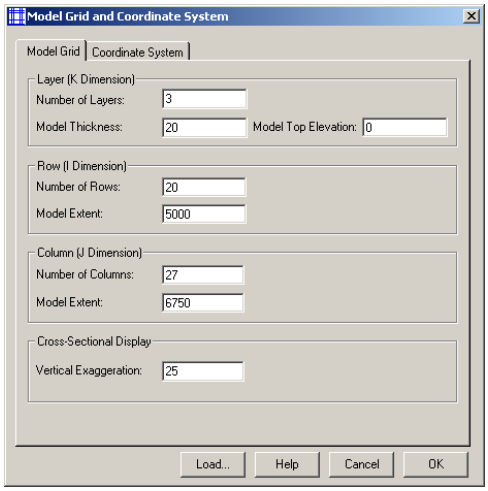


Fig. 4.49. The Model Grid and Coordinate System dialog box

You are now in the Grid Editor. To help visualize the problem we can overlay a DXF file as a map, which gives us the locations of the boundaries and the pumping wells.

► To load a map

1. Select *Options* | *Map* to open the Map Options dialog box.
2. Right-click on the first DXF File field to bring up the Map Files dialog box and then select the file BASEMAP.DXF from the folder \examples\tutorials\tutorial3\.
3. Check the box at the front of the DXF File field. The map will be displayed only if the box is checked.
4. Click *OK* to close the Map Options dialog box.
   You will see that it does not match the grid that you have generated. So, we need to move the grid to the proper position.

► To move the grid

1. Select *Options* | *Environment* to open the Environment Options dialog box.
2. In the Coordinate System tab, enter Xo = 200 and Yo = 6000, then click *OK* to close the dialog box.
3. Select *File* | *Leave Editor* or click the leave editor button .

4.3.1.3 Step 3: Refine the Model Grid

► To refine the model grid

1. Select *Grid* | *Mesh Size* to open the Grid Editor.

2. Refine the grid around each of the three wells by halving the size of the following rows and columns:
   Columns 8 through 14
   Rows 7 through 12
   The grid should now be refined around the wells and appear similar to Fig. 4.50.
3. Select *File* | *Leave Editor* or click the leave editor button .

4.3.1.4 Step 4: Assign Model Data

► To define the layer properties

1. Select *Grid* | *Layer Property* to open the Layer Property dialog box.
2. Make sure that for layer 1 the type is set to *1:unconfined,* and layers 2 and 3 are set to *3:confined/unconfined*. Note that MODFLOW requires horizontal hydraulic conductivity for layers of type 1 or 3, and transmissivity for layers of type 0 or 2. Refer to Section 2.4.2 (page 27) for details of the Layer Property dialog box.
3. Click *OK* to close the Layer Property dialog box.

► To define the model boundaries

1. *Select Grid* | *Cell Status* | *IBOUND (Modflow)*.
2. Click the button if the display mode is not Grid View.
3. Set no-flow boundaries in the first layer in the areas defined by the Granite and South Granite Hills.

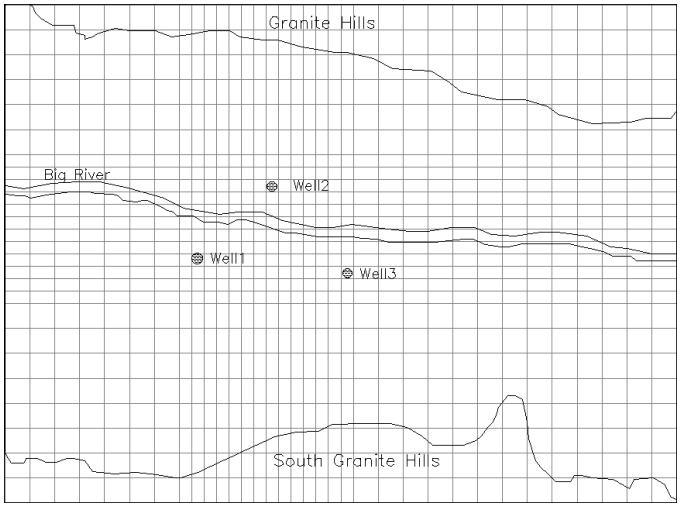


Fig. 4.50. Model grid after the refinement

4. Turn *layer copy* on by click the layer copy button .
   Layer Copy is on, if the layer copy button is sunk. The cell values of the current layer will be copied another layer, if you move to the other model layer while layer copy is on.
5. Move to the second layer and the third layer by pressing PgDn twice.
6. Set fixed-head boundaries (IBOUND = -1) in layer 3 at the west and east boundaries where the river enters and leaves the model area.
7. Copy the fixed-head boundaries from layer 3 to layer 1 by clicking the *Current Layer* edit field in the tool bar; typing in the layer number 1, and pressing the *Enter* key (remember that layer copy is still on). We do not need to specify fixed-head cells in the second layer, because the horizontal flow component in the silty layer is considered to be negligible. The model grid in layers 1 and 3 should look like Fig. 4.51. The model grid in layer 2 should look like Fig. 4.52.
8. Select *File* | *Leave Editor* or click the leave editor button .

The top of each aquifer slopes gradually from west to east. To save you entering this data, the top elevation of each aquifer has been saved in ASCII Matrix file.

► To specify the top elevation of each aquifer

1. Select *Grid* | *Top of Layers (TOP)*. **PM** will ask if you want to use the layer bottom elevations as the layer top elevations. Click *No*.
2. Click the button if the display mode is not Grid View.
3. Select *Value* | *Matrix* | *Load* to import \examples\tutorials\tutorial3\aq1top.dat as the elevation of the top of aquifer 1.
4. Move to Layer 2.

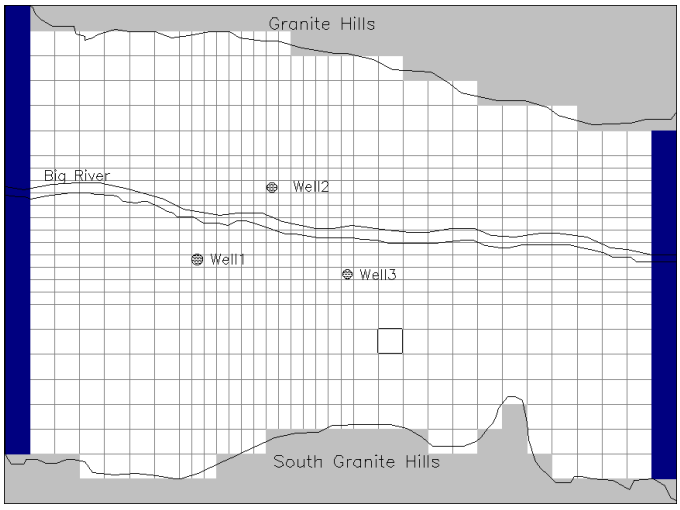


Fig. 4.51. Model grid of the 1st layer and 3rd layer

Fig. 4.52. Model grid of the 2nd layer

5. Select *Value* | *Matrix* | *Load* to import \examples\tutorials\tutorial3\aq2top.dat as the elevation of the top of aquifer 1.
6. Move to Layer 3.
7. Select *Value* | *Matrix* | *Load* to import \examples\tutorials\tutorial3\aq3top.dat as the elevation of the top of aquifer 1.
8. Select *File* | *Leave Editor* or click the leave editor button .

► To specify the bottom elevation of each aquifer

1. Select *Grid* | *Bottom of Layers (BOT)*. **PM** will ask if you want to use the Top of Layer 2 as the Bottom of Layer 1, and Top of Layer 3 as the Bottom of Layer 2. We will accept this.
2. Move to the layer 3 and select *Value* | *Reset Matrix* to set the elevation of the bottom of the layer 3 to 0.0 m.
3. Select *File* | *Leave Editor* or click the leave editor button .

Specification of the geometry of the system is now complete; all we need to do now is enter the physical parameters of the system.

► To specify the time parameters

1. Select *Parameters* | *Time*.
2. In the Time Parameters dialog box, change the *Simulation Time Unit* to DAYS and select *Steady State* in the *Simulation Flow Type* box.
3. Click *OK* to close the Time Parameters dialog box.

The groundwater flows naturally under a gentle gradient towards the river from both sets of hills and also in an easterly direction. The values of starting heads (which include the required values for the fixed-head cells) are saved in \examples\tutorials\tutorial3\t2sh.dat. We will import this file to the initial hydraulic head.

► To specify the initial & prescribed hydraulic heads

1. Select *Parameters* | *Initial & Prescribed Hydraulic Heads*.
2. Select *Value* | *Matrix* to open the Browse Matrix dialog box.
3. Click the button, select the file \examples\tutorials\tutorial3\t2sh.dat, and then click *OK*.
   The data will appear in the Browse Matrix dialog box, click *OK* to close this dialog box and return to the Data Editor. The data is now loaded into layer 1.
4. Turn on layer copy by pressing down the layer copy button.
5. Move to the second layer and the third layer. Now, the data of layer 1 is copied to the second and third layers.
6. Select *File* | *Leave Editor* or click the leave editor button .

► To specify the horizontal hydraulic conductivity

1. Select *Parameters* | *Horizontal Hydraulic Conductivity*.
2. Use *Value* | *Reset Matrix* to enter the following data for each layer,
   Layer 1: 5.0 m/day
   Layer 2: 0.5 m/day
   Layer 3: 2.0 m/day
3. Select *File* | *Leave Editor* or click the leave editor button .

► To specify the vertical hydraulic conductivity

1. Select *Parameters* | *Vertical Hydraulic Conductivity*.
2. Use *Value* | *Reset Matrix* to enter the following data for each layer,
   Layer 1: 0.5 m/day
   Layer 2: 0.05 m/day
   Layer 3: 1.0 m/day
3. Select *File* | *Leave Editor* or click the leave editor button .

► To specify the effective porosity

1. Select *Parameters* | *Effective Porosity*.
   The effective porosity is used in PMPATH, which will be used to define the capture zones of the pumping wells.
2. Use *Value* | *Reset Matrix* to enter the following data for each layer,
   Layer 1: 0.2
   Layer 2: 0.25
   Layer 3: 0.25

3. Select *File* | *Leave Editor* or click the leave editor button .

► **To specify the well data**

1. Select *Models* | *Modflow* | *Well*.
2. Click the button if the display mode is not Grid View.
3. Switch to Layer 3 by pressing the PgDn key twice.
4. Move the grid cursor to Well 1, press *Enter* or right-click, and set the pumping rate to -500 [m^3/day].
5. Repeat the above step with Well 2 and Well 3.
6. Select *File* | *Leave Editor* or click the leave editor button .

The last step before running the steady-state simulation in this tutorial is to specify river data, which is a little difficult to set up. MODFLOW requires that the river data (i.e. river stage, river bottom elevation, and riverbed conductance) be specified to each model cell. The riverbed conductance is defined as

$$C_{riv} = \frac{K_{riv} \cdot L \cdot W_{riv}}{M_{riv}} \tag{4.4}$$

where,
C_{riv} = hydraulic conductance of the riverbed [L^2T^{-1}]
K_{riv} = hydraulic conductivity of the riverbed sediment [LT^{-1}]
L = length of the river within a cell [L]
W_{riv} = width of the river within a cell [L]
M_{riv} = thickness of the riverbed within a cell [L]

Entering the river data on a cell-by-cell basis is sometimes very cumbersome. Fortunately, pmp provides a Polyline input method, which dramatically facilitates the data input process. We will use this input method to specify the river data.

► **To specify the river data**

1. Select *Models* | *Modflow* | *River* to open the Data Editor.
2. Click the button if the display mode is not Grid View.
3. Click the button to switch to the Polyline input method.
4. Left-click on the upstream end of the river to anchor one end of the polyline.
5. Move the mouse pointer along the trace of the river and left-click to anchor another vertex of the polyline.
6. Repeat steps 4 and 5 until the polyline looks similar to Fig. 4.53, then click on the latest vertex again to complete to polyline. While drawing the polyline, you may press the right mouse button to abort.
7. Right-click on the first vertex of the polyline on the upstream side to open a River Parameters dialog box and enter the values as shown in Fig. 4.54, then click *OK* to close the dialog box.

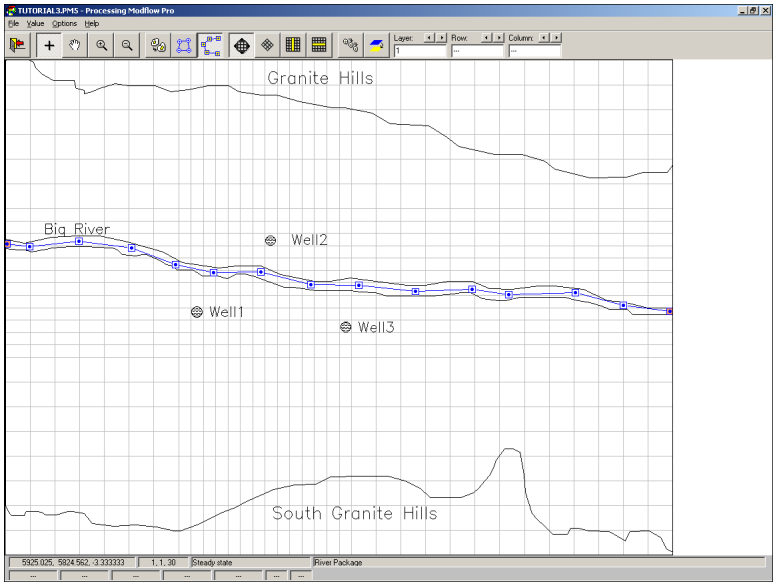


Fig. 4.53. Define the river using a polyline

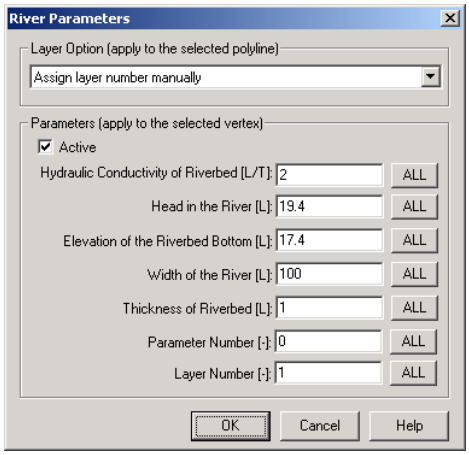


Fig. 4.54. Parameters of the upstream vertex

8. Right-click on the last vertex of the polyline on the downstream side to open a River Parameters dialog box and enter the values as shown in Fig. 4.55, then click *OK* to close the dialog box.
   The parameters specified to the vertices are used to calculated the cell properties along the trace of the polyline. Refer to Section 2.6.1.8 (page 51) for details.
9. Select *File* | *Leave Editor* or click the leave editor button .

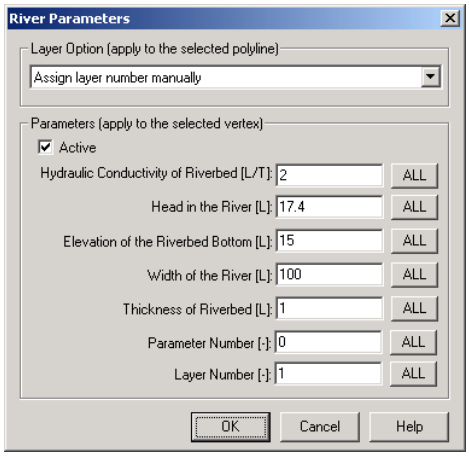


Fig. 4.55. Parameters of the downstream vertex

4.3.1.5 Step 5: Perform steady-state flow simulation

► To run the flow simulation

1. Select *Models* | *Modflow* | *Run*.
2. Click OK in the Run Modflow dialog box to generate the required data files and to run MODFLOW, you will see a DOS window open and MODFLOW perform the iterations required to complete the flow simulation.
3. Press any key to exit the DOS Window.

4.3.1.6 Step 6: Extract and view results

► To generate contour maps of the calculated heads

1. Select *Tools* | *2D Visualization* to display the Result Selection dialog box (Fig. 4.56).
2. Click *OK* to select the default result type *Hydraulic Head*.
   PM displays the model grid and sets 10 contour levels ranging from the lowest to the highest head value.
3. Select *Options* | *Environment* to customize the appearance of the contours. The contour map for the first model layer should look similar to that in Fig. 4.57.

► To delineate the capture zones of the pumping wells

1. Start PMPATH by selecting *Models* | *PMPATH (Advective Transport)*.
   PMPATH will load the current model automatically. We will place particles around the pumping wells and examine their 10-year capture zones.
2. Move to Layer 3 by pressing the PgDn key twice.

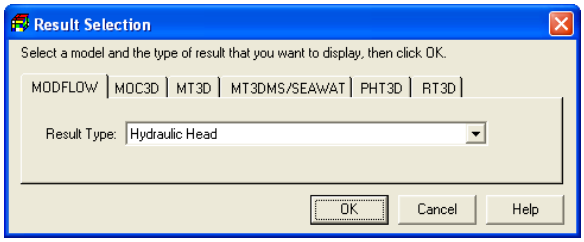


Fig. 4.56. The Result Selection dialog box

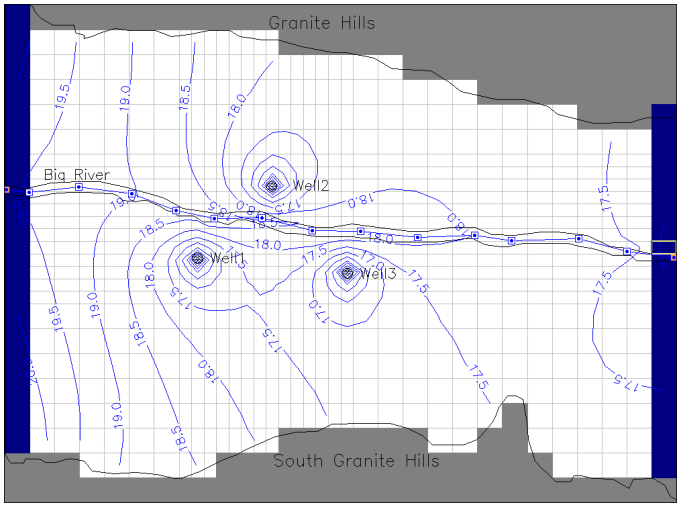


Fig. 4.57. Steady state hydraulic head distribution in the first model layer

3. Click on the + button and drag a small box around the cell containing Well 1 by holding down the left mouse button and moving the mouse.
4. When you release the mouse button, the Add New Particles dialog box appears. In the *Particles on circles* group, set the number of particles to 15, the radius R = 80, and the number of planes NK = 3.
5. Click the *Properties* tab and change the color of new particles to Blue.
6. Click *OK* to close the Add New Particles dialog box.
7. Use a similar procedure to add particles around Well 2 and Well 3. Assign a different color (say Green and Black) to each of these particle groups.
8. Select *Options* | *Environment* to open the Environment Options dialog box for setting up the display of the hydraulic heads contours and cross sections.
9. Click the *Contours* tab, check the *Visible* box, and click the *Restore Defaults* button to get standard settings.
10. Click the *Cross Sections* tab, check the *Visible* and *Show grid* boxes, and set *Exaggeration* = 25, *Projection Row* = 15 and *Projection Column* = 9.

11. Click *OK* to close the Environment Options dialog box.
    The hydraulic head contours for layer 3 and cross sections showing the location of the particles should appear.
12. Select *Options* | *Particle Tracking (Time)* to open the Particle Tracking (Time) Properties dialog box for setting up the particle tracking parameters. In the *Tracking Steps* group, change the (time) unit to years, step length to 10, and maximum number of steps to 200.
13. Click *OK* to close the Particle Tracking (Time) Properties dialog box.
14. Start the backward particle tracking by clicking on the ◄ button.
    You can easily see that the flowlines intersect with the river in numerous places (Fig. 4.58).

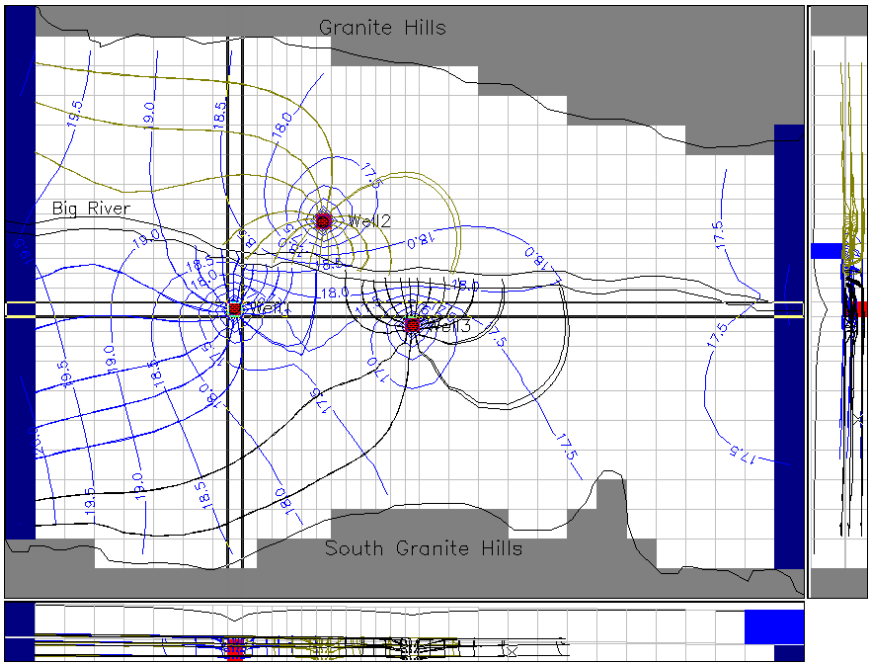


Fig. 4.58. Steady state hydraulic head distribution in the 3rd model layer and capture zones of the pumping wells

► To run forward particle tracking

We will now introduce a contaminant source upstream of Well 2 and see how far the contamination moves through the steady state flow field after 75, 100 and 125 years.

1. Since the contamination is a surface source we need to place the particles in layer 1. If you aren't already in Layer 1 change to it by using the PgUp key.

2. To place the particles on the ground surface, drag a box around the cell [1, 5, 6].

3. In the *Cell Faces* tab of the Add New Particles dialog box you will notice that the figure defines the various faces of an individual cell, since the contamination is a surface source we only want to place particles on cell face 5.
4. Click the *Particles* tab and set the number of particles on *Face 5* to NI=4 and NJ=4, and set all the other values to 0.
5. Click *OK* to close the Add New Particles dialog box.
6. Open the Particle Tracking (Time) Properties dialog box by selecting *Options* | *Particle Tracking (Time)*.
7. In the *Tracking Steps* group, change the (time) unit to years, step length to 1, and maximum number of steps to 75. When finished, click OK to close the dialog box.
8. Start the backward particle tracking by clicking on the button.
9. Repeat the above for Maximum number of steps of 100 and 125. The plot generated after 125 steps should look similar to Fig. 4.59.

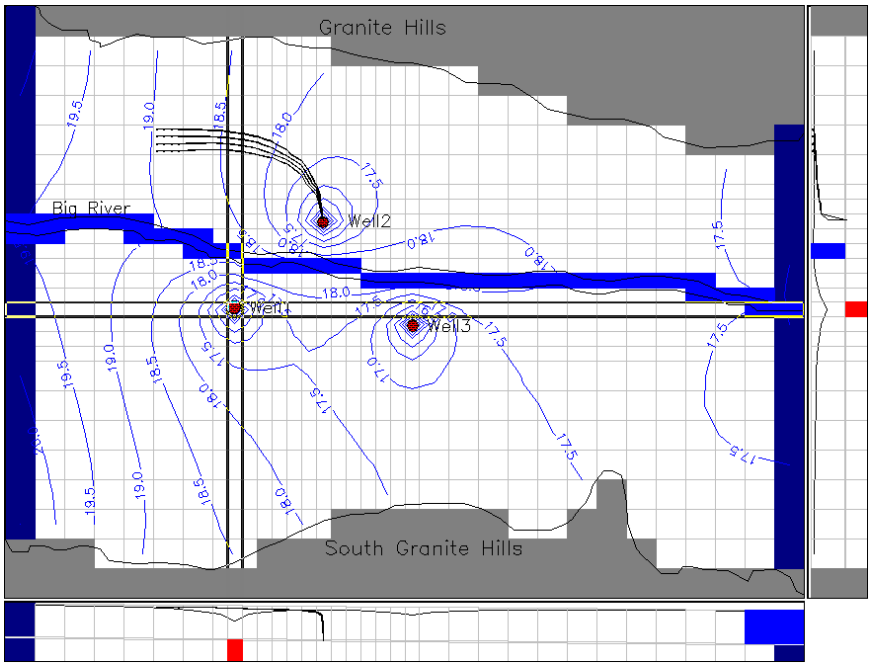


Fig. 4.59. 125-year streamlines; particles are started at the cell [6, 5, 1] and flow towards Well 2

5

Examples and Applications

The examples contained in this chapter are intended to illustrate the use of **PM** and the supported programs. The description of each problem is divided into three parts. It starts out with Folder, where you can find the ready-to-run model, for example *pmdir*\examples\basic\basic1\ (*pmdir* is the installation folder of **PM**). Next, you'll find a discussion of the problem, and finally you will find the simulation results.

5.1 Basic Flow Problems

5.1.1 Determination of Catchment Areas

Folder: *pmdir*\examples\basic\basic1

Overview of the Problem

Fig. 5.1 shows a part of an unconfined aquifer. The extent of the aquifer to the North and South is assumed to be unlimited. The aquifer is homogeneous and isotropic with a measured horizontal hydraulic conductivity of 0.0005 m/s and an effective porosity of 0.1. The elevations of the aquifer top and bottom are 15 m and 0 m, respectively. The aquifer is bounded by a no-flow zone to the west. To the east exists a river, which is in direct hydraulic connection with the aquifer and can be treated as fixed-head boundary. The river width is 50 m and stage is 10 m. The mean groundwater recharge rate is 8×10^{-9} m/s. A pumping well is located at a distance of 1000 m from the river.

The task is to calculate the catchment area of the well and the 365-days-capture zone under steady-state flow conditions.

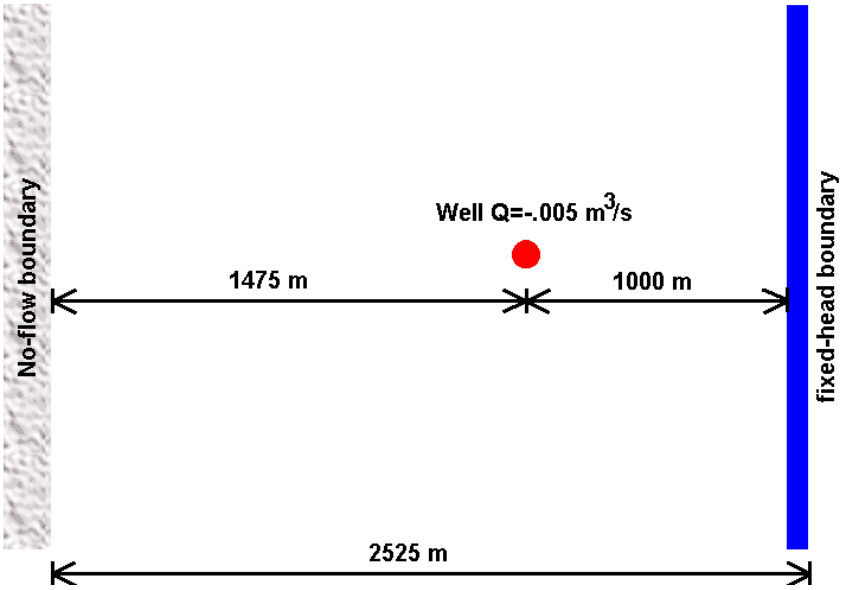


Fig. 5.1. Plan view of the model area

Modeling Approach and Simulation Results

The west boundary of the model is impervious and the river to the east is simulated by the fixed-head boundary condition (IBOUND = -1) with the initial hydraulic head at 10 m. There are no natural boundaries to the South and North, so we have to use streamlines as impervious boundaries. The distance of the selected streamline from the well must be large enough, so that the hydraulic head at these boundaries are not affected by the pumping well. This is the case if the total recharge in the chosen strip is considerably larger than the pumping rate of the well. Because of the symmetry of the system, we could use one-half of the model area only. To show the whole catchment area, we decided to use the entire model area.

The aquifer is simulated using a grid of one layer, 50 rows and 51 columns. A regular grid space of 50 m is used for each column and row. The layer type is 1: unconfined. Fig. 5.2 shows the contours, the catchment area, and the 365-days-isochrones of the pumping well using a 2D-approach, where the groundwater recharge is treated as a distributed source within the model cells and 50 particles are initially placed around the pumping well in the middle of the aquifer. If the groundwater recharge is applied on the groundwater surface (refer to RCH/EVT Tab, page 222), particles will be tracked back to the ground-water surface (Fig. 5.3). We can easily imagine that the size and form of the calculated catchment area depend on the boundary condition, recharge rate and the vertical position of the well screen, if the well is only partially penetrating. A discussion about the determination of catchment areas in two and three spatial dimensions can be found in Kinzelbach and others [71].

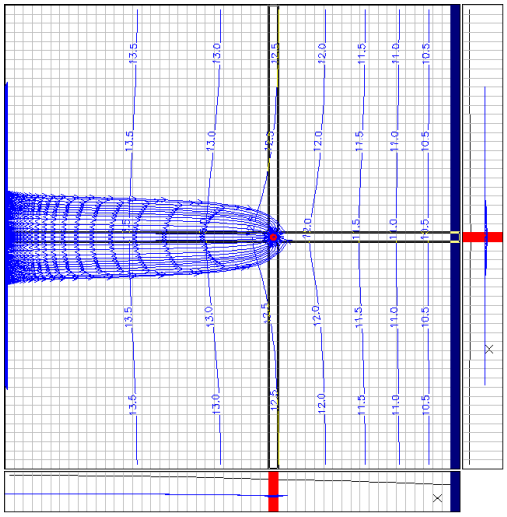


Fig. 5.2. Catchment area and 365-days isochrones of the pumping well (2D-approach: ground-water recharge is treated as distributed source within the model cells)

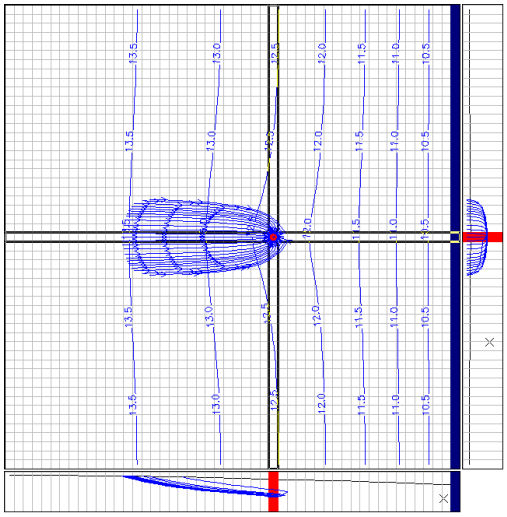


Fig. 5.3. Particles are tracked back to the groundwater surface by applying the groundwater recharge on the groundwater surface (3D-approach)

To delineate the catchment area of a pumping well in a 3D flow field, we must place enough particles around and along the well screen. Fig. 5.4 shows the catchment area calculated by PMPATH. First, 425 particles are placed around the well by using the Add New Particles dialog box (the settings are NI=5, NJ=5 on faces 5 and 6, and 25 particles on the circles with R=25 and NK=15 around the pumping well).

Then backward tracking is applied for a 100-years duration. Finally, the end points of the particles are saved by selecting *File* | *Save Particles As* in PMPATH. This file can be reloaded into PMPATH by selecting *File* | *Load Particles* to display the catchment area.

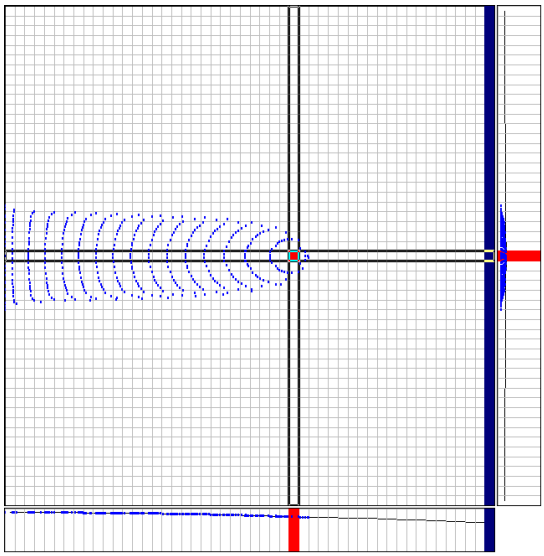


Fig. 5.4. Catchment area of the pumping well (3D-approach)

5.1.2 Use of the General-Head Boundary Condition

Folder: *pmdir*\examples\basic\basic2

Overview of the Problem

This simple example (Kinzelbach and Rausch [72]) demonstrates the use of the general-head boundary package of MODFLOW. A confined, homogeneous and isotropic aquifer is shown in Fig. 5.5. The aquifer is bounded by no-flow zones to the north and south. The hydraulic heads at the west and east boundaries are 12 m and 10 m, respectively. The transmissivity of the aquifer is T = 0.01 m^2/s. The aquifer has a constant thickness of 10 m.

The task is to calculate the head contours for the case that only the west part of the aquifer is modeled. The east boundary of the modeled part should be approached by using the general-head boundary.

Modeling Approach and Simulation Results

The aquifer is simulated using a grid containing 1 layer, 10 rows, and 16 columns. A regular grid spacing of 100 m is used for each column and row. The layer type is 0: confined and the Transmissivity flag in the Layer Options dialog box is User-specified. The initial hydraulic head is 12 m everywhere. While the west model boundary is simulated by the fixed-head boundary condition (IBOUND = -1) with

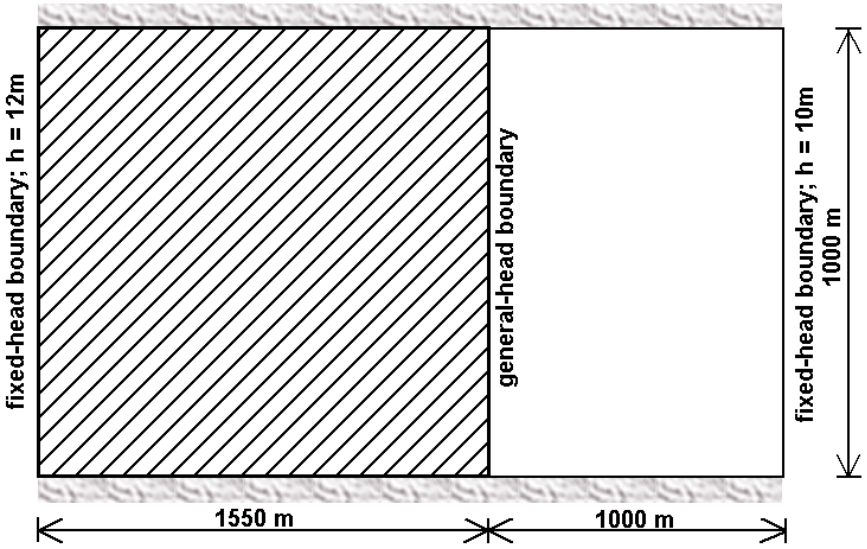


Fig. 5.5. Plan view of the model area

the initial head at 12 m, the east boundary is simulated by the general-head boundary (GHB) condition with the head h = 10 m. Analogous to the riverbed hydraulic conductance (equation 2.19), the hydraulic conductance term of each GHB cell is $C_{GHB} = K_{GHB} \cdot A/L$, where K_{GHB} is the (horizontal) hydraulic conductivity, L is the distance from the actual fixed-head boundary to the modeled GHB cell, and A is the area of the cell face, which is perpendicular to the groundwater flow in the unmodeled area. For this example $C_{GHB} = (T/10) \cdot (100 \cdot 10)/1000 = 0.001\, m^2/s$.

Fig. 5.6 shows the calculated contours. For comparison, the entire aquifer is modeled with the east and west fixed-head boundaries and the result is shown in Fig. 5.7. The model is saved in the folder *pmdir*\examples\basic\basic2a\.

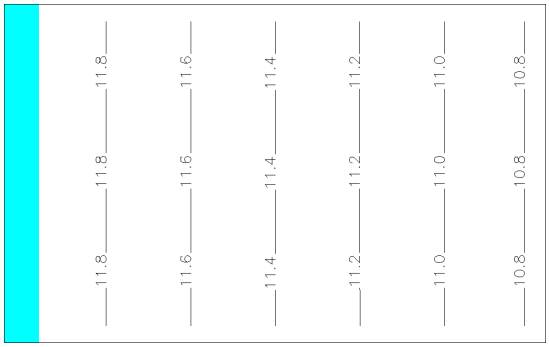


Fig. 5.6. Calculated head contours for the west part of the aquifer

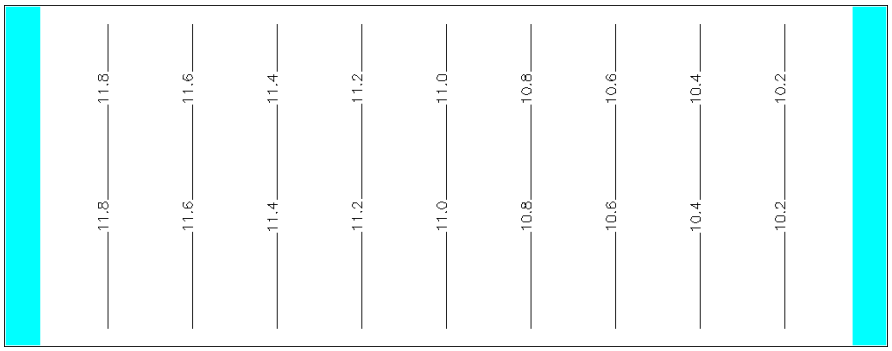


Fig. 5.7. Calculated head contours for the entire aquifer

5.1.3 Two-layer Aquifer System in which the Top layer Converts between Wet and Dry

Folder: *pmdir*\examples\basic\basic3

Overview of the Problem

This example is adapted from the the first test problem of the BCF2 package (McDonald and others [86]). In an aquifer system where two aquifers are separated by a confining bed, large pumping rates from the bottom aquifer can desaturate parts of the upper aquifer. If the pumping is discontinued, resaturation of the upper aquifer can occur.

Fig. 5.8 shows two aquifers separated by a confining unit. No flow boundaries surround the system on all sides, except that the lower aquifer discharges to a stream along the right side of the area. Recharge from precipitation is applied evenly over the entire area. The stream penetrates the lower aquifer; in the region above the stream, the upper aquifer and confining unit are missing. Under natural conditions, recharge flows through the system to the stream. Under stressed conditions, two wells withdraw water from the lower aquifer. If enough water is pumped, cells in the upper aquifer will desaturate. Removal of the stresses will then cause the desaturated areas to resaturate.

The task is to construct a model to compute the natural steady-state head distribution, and then calculate the head distribution under the stressed condition. When solving for natural conditions, the top aquifer initially is specified as being entirely dry and many cells must convert to wet. When solving for pumping condition, the top aquifer is initially specified to be under natural conditions and many cells must convert to dry.

Modeling Approach and Simulation Results

The model consists of two layers - one for each aquifer. Since horizontal flow in the confining bed is small compared to horizontal flow in the aquifers, and storage is not a factor in steady state simulations, the confining bed is not treated as a separate model layer. The effect of the confining bed is incorporated in the value for vertical leakance. Note that if storage in the confining bed were significant, transient simulations would require that the confining layer be simulated using one or more layers. The confining layer must also be simulated, if you intend to calculate pathlines with PMPATH or to simulate solute transport. A uniform horizontal grid of 10 rows and 15 columns is used. Aquifer parameters are specified as shown in Fig. 5.8.

Two steady state solutions were obtained to simulate natural conditions and pumping conditions. The steady state solutions were obtained through a single simulation consisting of two stress periods. The first stress period simulates natural conditions and the second period simulates the addition of pumping wells with extraction rates of 30000 ft^3/d ($\simeq$ 850 m^3/d). The simulation is declared to be steady state, so no storage values are specified and each stress period requires only a single "time

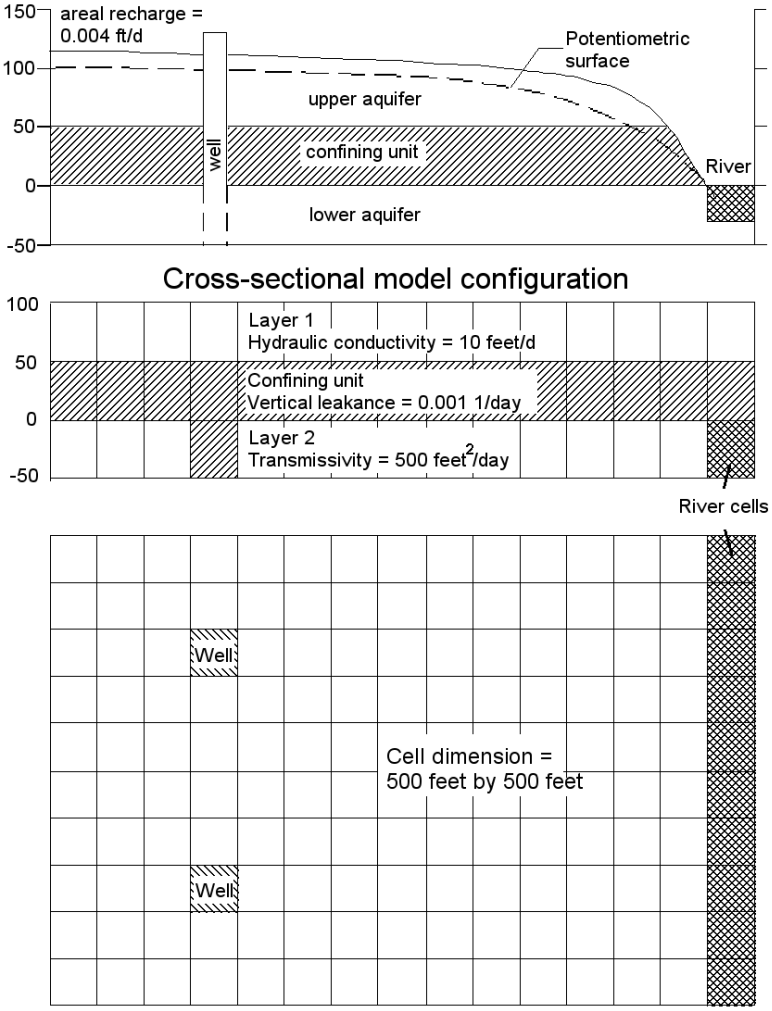


Fig. 5.8. Configuration of the hypothetical model (after McDonald and others [86])

step" to produce a steady state result. The PCG2 Package is used to solve the flow equations for the simulations.

Determination of the wetting threshold THRESH (see *Modflow | Wetting Capability*) often requires considerable effort. The user may have to make multiple test runs trying different values in different areas of the model. In many cases, positive THRESH values may lead to numerical instability and therefore the user should try negative THRESH values first.

5.1.4 Water-Table Mount resulting from Local Recharge

Folder: *pmdir*\examples\basic\basic4\

Overview of the Problem

This example is adapted from the the first test problem of the BCF2 package (McDonald and others [86]). Localized recharge to a water table aquifer results in formation of a ground water mound. For example, a ground water mound may form in response to recharge from infiltration ponds commonly used to artificially replenish aquifers or to remove contamination by filtration through a soil column. If the aquifer has low vertical hydraulic conductivity or contains interspersed zones of low hydraulic conductivity, it may be necessary to simulate the aquifer using multiple model layers in which the mound crosses more than one layer.

The conceptual model consists of a rectangular, unconfined aquifer overlain by a thick unsaturated zone (Fig. 5.9). The horizontal hydraulic conductivity is 5 feet per day and vertical hydraulic conductivity is 0.25 feet per day ($\simeq 0.0762\ m/d$). A leaking pond recharges the aquifer, resulting in the formation of a ground water mound. The pond covers approximately 6 acres ($\simeq 23225 m^2$) and pond leakage is 12,500 cubic feet per day ($\simeq 354\ m^3/d$). The specific yield is 20 percent. The water table is flat prior to the creation of the recharge pond. The flat water table is the result of a uniform fixed head boundary that surrounds the aquifer.

The task is to calculate the water table under the steady-state condition and the formation of the groundwater mound over time.

Modeling Approach and Simulation Results

Because of the symmetry, heads are identical in each quadrant of the aquifer, and there is no flow between quadrants; therefore, only one quarter of the system needs to be simulated. The problem is simulated using a grid of 40 rows, 40 columns, and 14 layers (Fig. 5.9). A uniform horizontal grid spacing of 125 feet ($\simeq 38.1\ m$) is used, and each layer is 5 feet ($\simeq 1.52\ m$) thick. The pond is in the upper left corner of the grid. The boundaries along row 1 and column 1 are no flow as a result of the symmetry. A fixed head boundary of 25 feet ($\simeq 7.62\ m$) is specified along row 40 and column 40 for layers 10 – 14; a no flow boundary is assigned along row 40 and column 40 for layers 1 – 9. Without the recharge from the pond, layers 1 – 9 are dry, and the head in all the cells of layers 10 – 14 is 25 feet. Recharge from the pond is applied to the horizontal area encompassed by rows 1 through 2, and columns 1 through 2. The recharge option "Recharge is applied to the highest active cell" is used so that recharge will penetrate through inactive cells down to the water table. The specific recharge rate of 0.05 foot per day ($\simeq 0.0152\ m/d$) simulates leakage of 3,125 cubic feet per day ($\simeq 88.5\ m^3/d$) through one quarter of the pond bottom, a simulated area of 62,500 square feet ($\simeq 5806 m^2$).

Reasonable solutions to the ground water mounding problem can be obtained in two steady state simulations by using the PCG2 solver. In the first simulation, dry

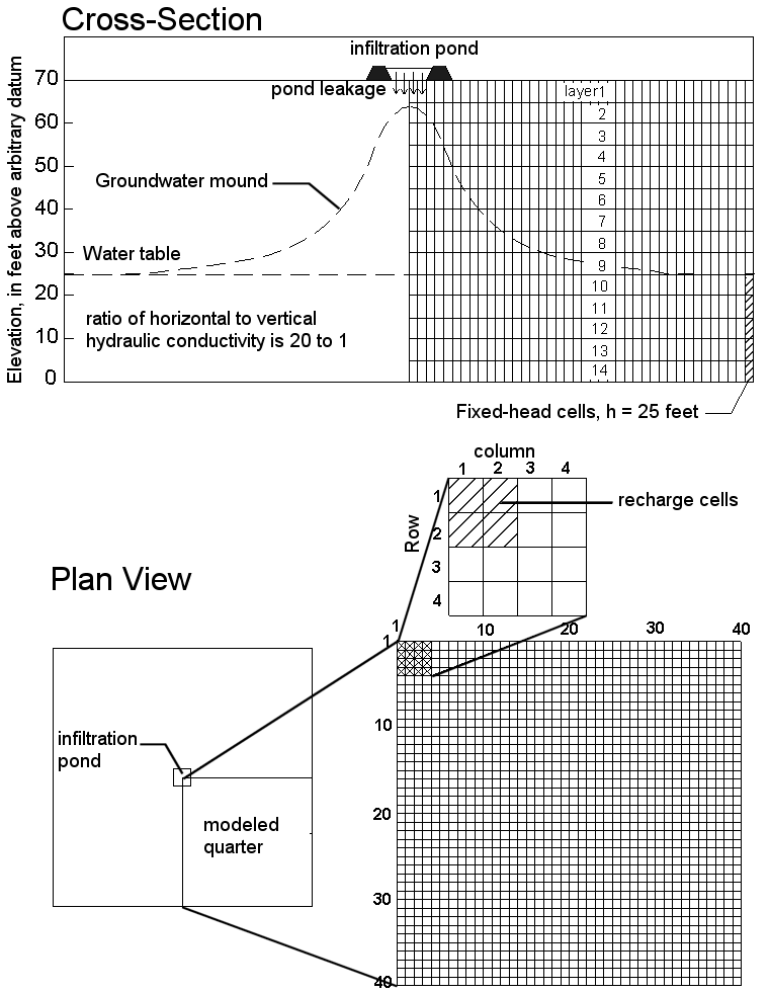


Fig. 5.9. Hydrogeology and model grid configuration

cells are converted to wet by comparison of the wetting threshold THRESH to heads in underlying cells only, which is indicated by a negative value of THRESH. The wetting iteration interval is 1 and THRESH is 0.5 foot, which means that the wetting threshold is 10 percent of the thickness of a cell. In the second simulation, wetting of cells is based on comparison to heads both in horizontally adjacent and underlying cells (THRESH is positive). A wetting iteration interval of 2 and a THRESH of 1.5 feet are used in order to prevent continued oscillation between wet and dry for some cells. Due to the steepness of the head gradient and the grid discretization, the head difference between adjacent horizontal cells is generally much larger than the head difference between adjacent vertical cells along the mound. For example, the cell at layer 4, row 3, and column 4 is supposed to be dry even though the head

in the horizontally adjacent cell in column 3 is 1.4 feet above the bottom of the layer. The vertical head difference between cells in this part of the model is much less; the difference between the head at the cell in layer 4, row 3, column 3 and the cell below is only 0.05 foot. Thus, the neighboring cell to the right is repeatedly and incorrectly converted to wet during the solution process if horizontal wetting is used with a wetting threshold of 0.5 foot. The larger wetting threshold and wetting iteration interval used in the second simulation allow convergence to occur, but only after many iterations. In this simulation, head in adjacent vertical cells is the best indicator of when a dry cell should become wet.

The formation of the groundwater mound over time can be obtained with a transient simulation. The transient simulation is run for one stress period with a length of 500,000 days. The stress period is divided into 50 time steps with a time step multiplier of 1.3. The first time step is 0.3 days, and the last time step is 115,385 days. The specific yield is 20 percent and the confined storage coefficient is 0.001. The PCG2 solver is used and cells are activated by comparison of the wetting threshold to heads in underlying cells. The head change criterion for closure is 0.001 foot and the residual change criterion is 10,000 cubic feet, the wet-ting threshold is 0.5 foot, the wetting factor is 0.5, and the wetting iteration interval is 1. Fig. 5.10 shows simulated water table heads along row 1 at several times during the transient simulation. Steady state conditions were reached at the 44th time step of the transient simulation as indicated by storage flow terms being zero (see the simulation listing file OUTPUT.DAT).

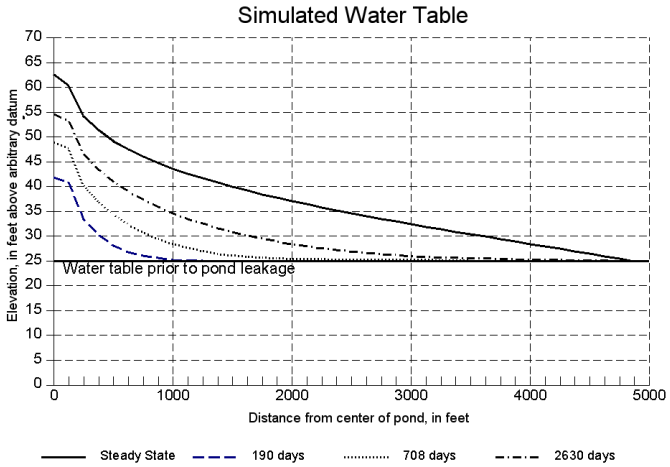


Fig. 5.10. Simulated water-table along row 1 beneath a leaking pond after 190, 708, 2630 days and steady state conditions

5.1.5 Perched Water Table

Folder: *pmdir*\examples\basic\basic5\

Overview of the Problem

This example is adapted from the the third test problem of the BCF2 package (McDonald and others [86]). Contrasts in vertical hydraulic conductivity within the unsaturated zone can provide a mechanism for the formation of perched ground water tables. The conceptual model is rectangular and consists of three geohydrologic units. The upper and lower units have higher hydraulic conductivities than the middle unit (Fig. 5.11). There is a regional water table in which the head is below the bottom of the middle unit. Natural recharge occurs over the entire area at a rate of 0.001 foot per day. This recharge can percolate through the two upper units without the formation of a water table above the middle because the vertical hydraulic conductivity of this unit is 0.002 foot per day.

Recharge at a rate of 0.01 foot per day from a pond covering 6 acres ($\simeq 23225\ m^2$) will cause a perched ground water body to form in the top two units. The total pond leakage is about 2,360 cubic feet per day ($\simeq 66.8\ m^3/d$). The perched water table spreads out over an area much larger than the area covered by the pond. This has an impact on the distribution of recharge to the lower unit.

The task is to calculate the long term head distribution resulting from the pond recharge.

Modeling Approach and Simulation Results

Because of the rectangular symmetry of the system, there is no flow between quadrants. Therefore, only one quarter of the system must be simulated. The problem is simulated using a grid of 50 rows, 50 columns, and 2 model layers. A uniform grid spacing of 16 feet is used. The recharge pond is in the upper left corner of the grid; the quarter of the pond that is simulated occupies a square area that is 16 rows long and 16 columns wide. The boundaries along row 1 and along column 1 are no flow boundaries as a result of the symmetry.

Model layer 1 simulates the upper geohydrologic unit and is assigned a hydraulic conductivity of 5 feet per day. The bottom of layer 1 is at an elevation of 20 feet. The lower geohydrologic unit is simulated as model layer 2. This layer is simulated as a confined/unconfined layer with constant transmissivity (layer type 2). The top and bottom elevations of layer 2 are set at 10 and 0 feet, respectively. Because the head in this layer is always below the layer top, the flow from above is limited as described by McDonald and Harbaugh ([85], p. 5 – 19). Thus, there is no direct hydraulic connection between the perched layer and the lower layer, but the perched heads have a direct impact on the recharge into the lower layer.

All cells in layer 2 are assigned a constant head of 1 foot because there is no need to simulate heads in this layer for the purpose of estimating recharge. The middle geohydrologic unit is not simulated as a separate model layer because it is assumed

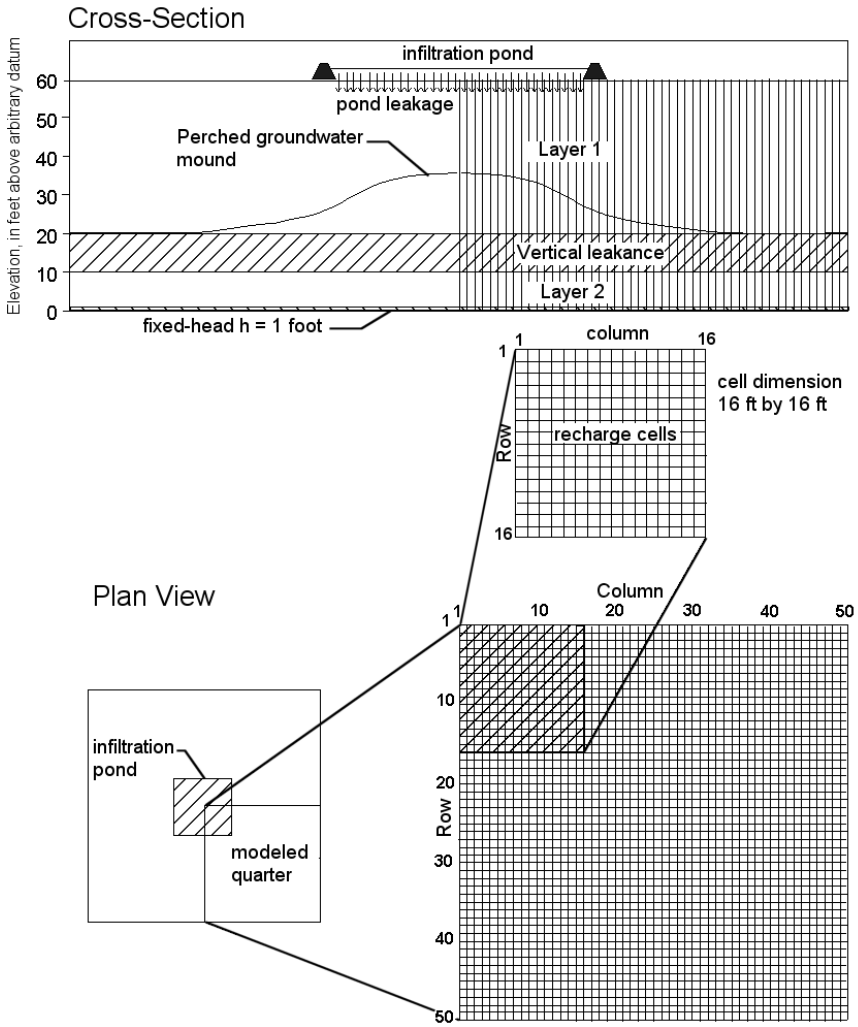


Fig. 5.11. Hydrogeology and model grid configuration

that horizontal flow and storage effects are negligible. This unit is represented by the value for vertical leakance between model layers 1 and 2. The vertical leakance is assumed to be 0.0002 per day. In areas not covered by the pond, recharge is applied areally at a rate of 0.001 foot per day to simulate natural re-charge. The recharge option ”Recharge is applied to the highest active cell” is used so that recharge will penetrate through inactive cells to the water table. A recharge rate of 0.01 foot per day is applied to the area covered by the pond.

A steady state simulation is performed to simulate the formation of a perched water table. Solution of the flow equation is obtained using the SIP solver. Starting

hydraulic head in layer 1 under the pond is set at 21 feet. All other cells in layer 1 initially are specified as no flow cells. The wetting iteration interval, THRESH, and wetting factor are set at 2 iterations, 1.0 foot, and 0.5 foot, respectively (see *MODFLOW | Wetting Capability*). A positive value of THRESH indicates that horizontally adjacent cells can cause dry cells to become wet. This is the only way for cells in layer 1 to become wet because heads in layer 2 are always below the bottom of layer 1.

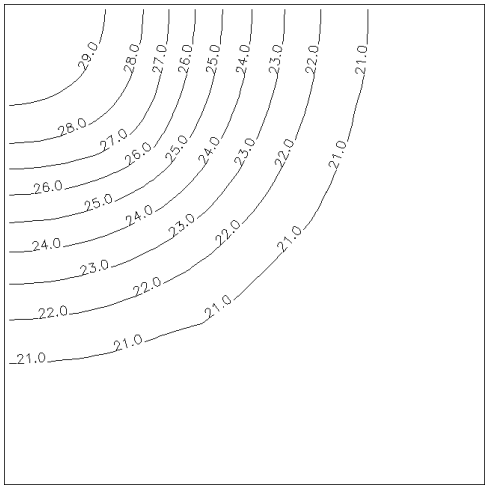


Fig. 5.12. Simulated steady state head distribution in layer 1

5.1.6 An Aquifer System with Irregular Recharge and a Stream

Folder: *pmdir*\examples\basic\basic6

Overview of the Problem

This example is adapted from the first test problem of the Streamflow Routing (STR1) package [98]. Results from the STR1 Package were compared to results from an analytical solution developed by Oakes and Wilkinson [90]. An idealized aquifer with a river flowing through the middle was chosen and is shown in Fig. 5.13. The width of the aquifer perpendicular to the river was 4,000 ft on each side, while the length parallel to the river was 13,000 ft. Assumptions used in both the analytical solution and the model simulation include:

1. The lateral boundaries of the aquifer are impermeable (no flow is allowed).
2. The rocks beneath the aquifer are impermeable.
3. The river penetrates the entire depth of the aquifer and has vertical banks.
4. The river is not separated from the aquifer by any confining material.

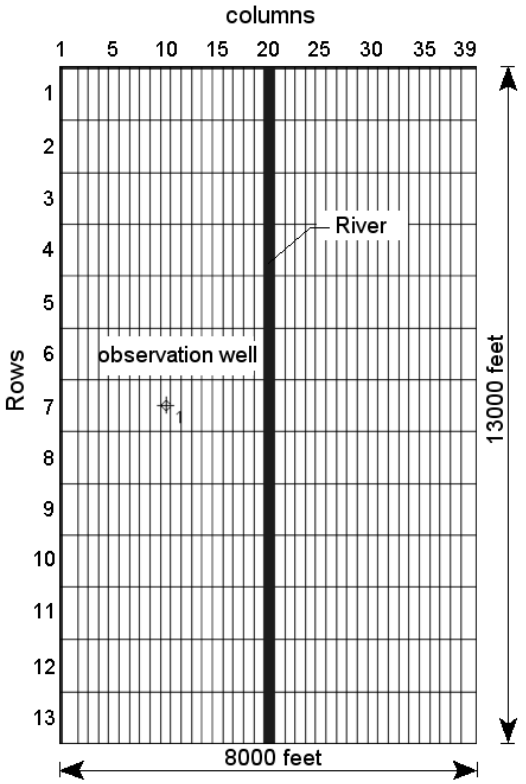


Fig. 5.13. Configuration of the model grid and the location of the observation well

5. The transmissivity and storage coefficient are constant throughout the aquifer and remain constant in time.
6. The aquifer is confined and Darcy's Law is valid.
7. The flow of groundwater is horizontal.
8. The water level in the river is constant along its length and with time.
9. The infiltration of recharge to the aquifer is instantaneous (no delay between the time precipitation infiltrates the surface until it reaches the water table).
10. The discharge from the aquifer is only to the river.

Transmissivity of the aquifer used for both the analytical solution and in the model simulation was 3,200 ft^2/d (3.45×10^{-3} m^2/s). The storage coefficient is 0.20. Because the river is assumed to be fully penetrating and the aquifer is not separated from the river by any confining material, the streambed conductance value was assumed equal to the transmissivity of the aquifer (in this example, the width of the river is assumed equal to the depth of the aquifer) times the length of the river in each cell (1,000 ft) divided by an assumed l foot thickness of the riverbed. Actually, any large streambed conductance value can be used as long as the head value in the model cell containing the river remains constant during the simulation. Varying the streambed conductance value shows that for this problem, streambed conductance values greater than 10 ft^2/d produce nearly the same results. Annual recharge to the aquifer is 1.5 ft. However, the daily recharge rate varied according to a sinusoidal distribution for the first 180 days, while no recharge was allowed for the following 180 days. The distribution of the recharge over time is shown in Fig. 5.14.

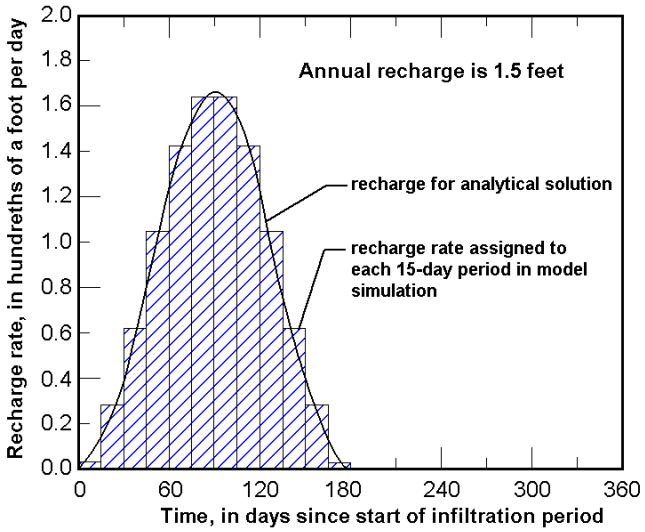


Fig. 5.14. Distribution of recharge used for analytical solution and the model (after Prudic [98])

Modeling Approach and Simulation Results

The aquifer is simulated using one model layer. Specification of the elevations of layer top and bottom are not necessary, because the layer is confined and transmissivity and confined storage coefficient are specified directly (as defined in the Layer Property dialog box). The sinusoidal distribution of the recharge rate was divided into 15 day intervals for the model simulation and the rate for the middle of each interval was used as input value. The distribution used in the simulation is also shown in Fig. 5.14. A total of six 360 day infiltration periods (144 stress periods, each with a length of 15 days) was used in the simulation. The first five 360-day infiltration periods were computed to allow the model to reach a stable yearly cycle because the starting water level for each model cell was not known. Results of the model simulation from the sixth infiltration period are compared to the results from the analytical solution for an observation well 2,000 ft from the river (Fig. 5.15). The coordinates of the observation well are given in the Head Observation dialog box. The Streamflow Routing package is not really needed to simulate this condition, as the river could have been represented using fixed-head or river cells. The same results can be obtained using the River pack-age. The simulation was done to determine whether the STR1 package correctly accumulates flow from the aquifer into the stream.

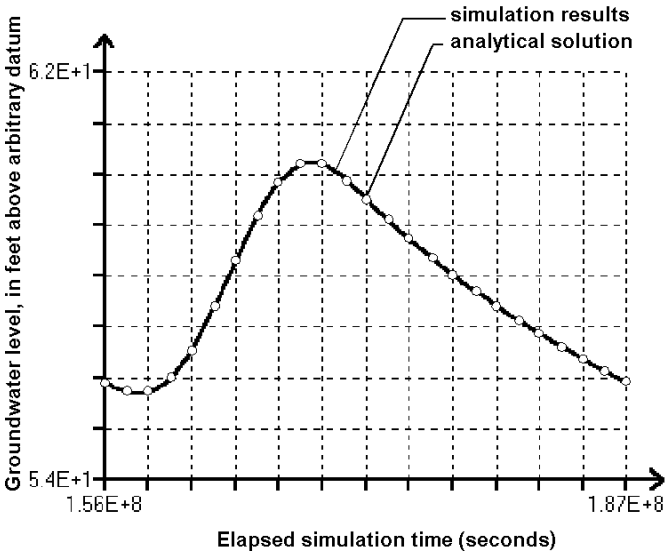


Fig. 5.15. Comparison of simulation results to analytical solution developed by Oakes and Wilkinson [90]

5.1.7 Flood in a River

Folder: *pmdir*\examples\basic\basic7\

Overview of the Problem

This example is adapted from the second test problem of the STR1 package [98]. The function of the STR1 package that computes the head in the stream as well as changes in flows to and from the aquifer was compared to an analytical solution developed by Cooper and Rorabaugh [28]. The model grid used in the previous example was also used in this model. The aquifer properties and assumptions are the same as those used in the previous example, except for assumptions 8 – 10, which are replaced with the following assumptions: (1) The recharge to the aquifer is only from the river as river stage increases with time, and (2) The discharge from the aquifer is only to the river as river stage decreases with time.

The analytical solution from Cooper and Rorabaugh ([28], pp. 355 – 358) is applicable for the case where the lateral boundary is at infinity (referred to by Cooper and Rorabaugh as semi-infinite). The impermeable boundary assigned at 4,000 ft for this model is of sufficient distance from the river in order not to interfere with the results. A flood in the river was simulated for a 30 day period.

The procedure used to calculate the distribution of streamflow for the 30 day period and for 60 days following the flood was first to calculate a distribution of river stage using equation 71 in Cooper and Rorabaugh ([28], p. 355), assuming a maximum flood stage of 4 ft above the initial river stage. The streamflow distribution (Fig. 5.16) was calculated from the river stage distribution. The river has a width of 100 ft, a dimensionless roughness coefficient of 0.02377 and a slope of 0.0001. A constant C = 1.486 should be used for the simulation (see Equation 2.26).

Modeling Approach and Simulation Results

Streamflow for the first 30 days was divided into l day periods for simulation. Fig. 5.17 shows the computed river stage. The simulation results are the same as the manually calculated river stage values using equation 71 of Cooper and Rorabaugh ([28], p. 355). Detailed discussion on the analytical and numerical results can be found in Prudic [98]. Results of varying both the number of columns and the length of stress periods used to simulate the flood wave indicate that both the number of columns and the length of the time step are important in exactly duplicating the analytical solution.

A groundwater flow model with the Streamflow Routing package has an advantage over analytical solutions because it can be used to simulate complex systems. An example (Folder: *pmdir*\examples\basic\basic7a\) containing a stream system (Fig. 5.18) is used to illustrate most of the features of the Stream-flow Routing package. The example assumes that an aquifer of 6,000 ft wide by 6,000 ft long is divided into six equally spaced rows and columns. The transmissivity of the aquifer is 0.08 ft^2/s. Recharge to the aquifer occurs only from stream leakage. The example in-

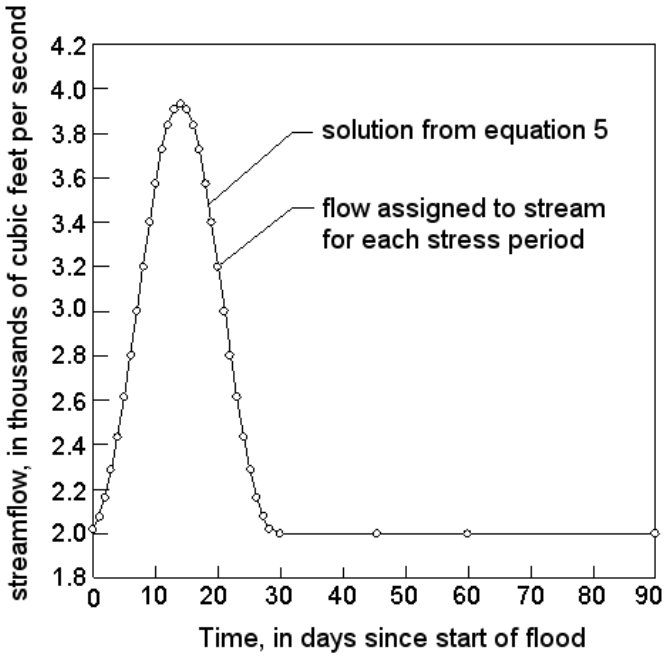


Fig. 5.16. Distribution of streamflow for a 30-day flood event used for the simulation (after Prudic [98])

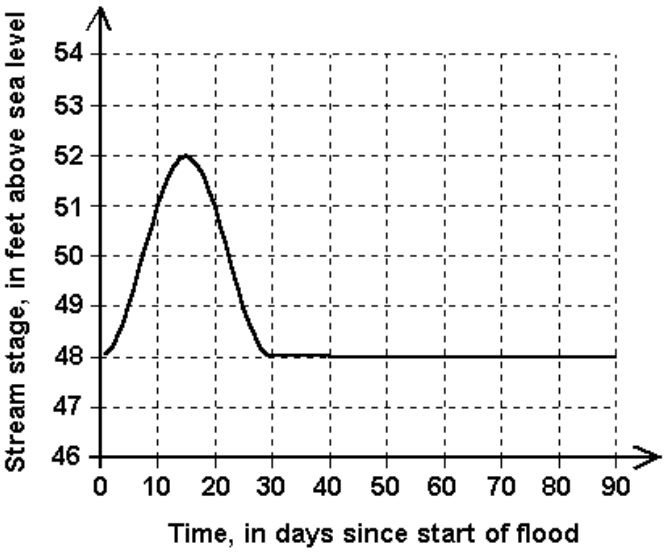


Fig. 5.17. Model calculated river stage

cludes 7 stream segments with totally 16 reaches. There is one diversion (segment 2) and two places where streams join (segments 2 and 4 join to make segment 5 and segments 3, 5, and 6 join to make segment 7). Stream stages are also computed for each reach. The streams range in width from 5 to 10 ft. Streambed conductance values also vary depending on the length and width of each stream reach. The hydraulic conductivity of the streambed is $4 \times 10^{-4} ft/s$.

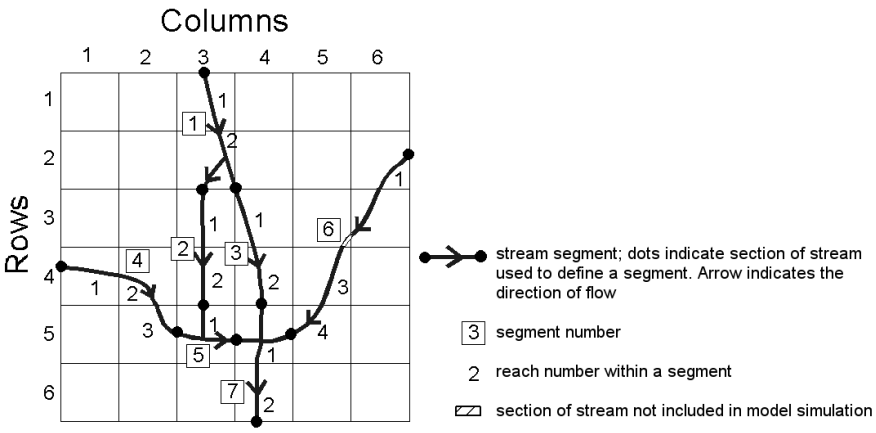

Columns
Rows
stream segment; dots indicate section of stream used to define a segment. Arrow indicates the direction of flow
segment number
reach number within a segment
section of stream not included in model simulation

Fig. 5.18. Numbering system of streams and diversions (after Prudic [98])

5.1.8 Simulation of Lakes

Folder: *pmdir*\examples\basic\basic8

Overview of the Problem

Fig. 5.19 shows an unconfined aquifer with the boundary conditions and the location of a planned opencast mining site. The aquifer is bounded by a no-flow zone to the north and to the south. To the west and east exist fixed-head boundaries with the hydraulic heads h = 100 m and 95 m; the elevations of the aquifer top and bottom are 100 and 0 m, respectively.

The aquifer is homogeneous and isotropic with a measured horizontal hydraulic conductivity of 0.0001 m/s and vertical hydraulic conductivity of 0.00001 m/s. The specific yield and effective porosity are assumed to be 0.25. The specific storage coefficient is 0.0001. In the final mining phase, the hydraulic head beneath the mining pit must be drawn down to the level of h = 21 m. Afterwards, the mining pit will be filled with water to form an artificial lake.

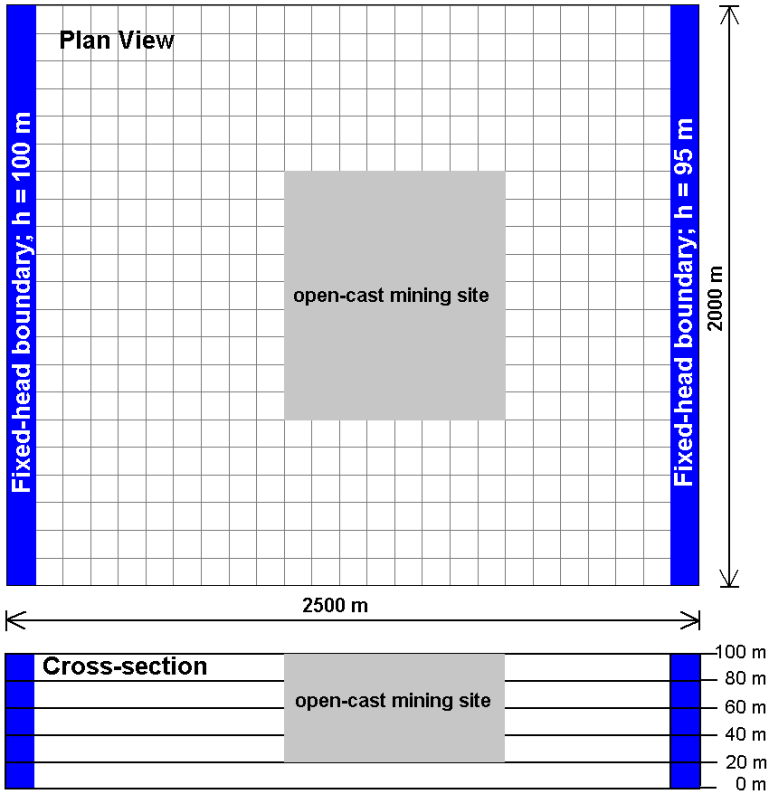


Fig. 5.19. Plan and cross-sectional views of the model area

The task is to

1. Construct a steady-state flow model and calculate the necessary abstraction rate (= inflow into the mining site) for holding the head at 21 m, and
2. Use the calculated steady-state head as the initial hydraulic head and calculate the temporal development curve of the water level (head vs. time) in the artificial lake for the case that the abstraction within the mining site is turned off.

Modeling Approach and Simulation Results

The aquifer is simulated using five model layers, 21 rows and 25 columns. The thickness of each model layer is 20 m. The elevation of the top of the first model layer is 100 m. A regular grid spacing of 100 m is used for each column and row. The layer type 3: confined/unconfined (transmissivity varies) is used for every layer.

For task #1, the cells within the mining pit in the 4th model layer are set as fixed-head cells with the initial hydraulic head of 21 m. The cells (of all 5 layers) at the west boundary are fixed-head cells with the initial head h = 100 m. The cells (of the layers 3 to 5) at the east boundary are fixed-head cells with the initial head h = 95 m. The initial hydraulic head values at all other cells have been set at 100 m. To ensure that there is no resistance to the groundwater flow within the mining pit, a very high value (say 1 m/s) is used for the vertical and horizontal hydraulic conductivities of the cells within the pit.

A steady-state flow simulation was performed. Fig. 5.20 shows the two cross-sections and the head contours of layer 4. It is obvious that the cells above the groundwater surface went dry. To calculate inflow into the mining pit, we select *Tools | Water Budget* to calculate the water budget by assigning zone 1 to the fixed-heads cells within the mining pit. The water budget for zone 1 in layer 4 should look like Table 5.1.8. The inflow rate to the constant head cells (mining pit) is 1.9428713E+00 m^3/s.

For task #2, all cells within the mining pit are set as active cells. The wetting capability of MODFLOW is turned on by selecting *Models | Modflow | Wetting Capability*. The wetting-iteration interval is 1, wetting factor is 0.5 and THRESH is -1 for all cells. The specific yield and effective porosity of all cells within the mining pit

Table 5.1 Volumetric budget for the entire model written by MODFLOW

Flow Term	**In**	**Out**	**In-Out**
STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
CONSTANT HEAD	0.0000000E+00	1.9428709E+00	1.9428709E+00
HORIZ. EXCHANGE	1.1840475E+00	0.0000000E+00	1.1840475E+00
EXCHANGE (UPPER)	0.0000000E+00	0.0000000E+00	0.0000000E+00
EXCHANGE (LOWER)	7.5882387E-01	0.0000000E+00	7.5882387E-01
WELLS	0.0000000E+00	0.0000000E+00	0.0000000E+00
DRAINS	0.0000000E+00	0.0000000E+00	0.0000000E+00
RECHARGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
ET	0.0000000E+00	0.0000000E+00	0.0000000E+00

(lake) are set to 1. Compared to the specific yield, the influence of the elastic storage coefficient within the lake is insignificant. Therefore, the specific storage coefficient Ss = 0.0001 is assigned to all cells. A transient flow simulation is performed for a stress period with the length of 3.15576E+08 seconds, 100 time steps and a time-step multiplier of 1.0. The temporal development curve of the water table at a measurement point located in the fourth layer within the lake, is shown in Fig. 5.21. The final stage in the lake is about 97.1 m.

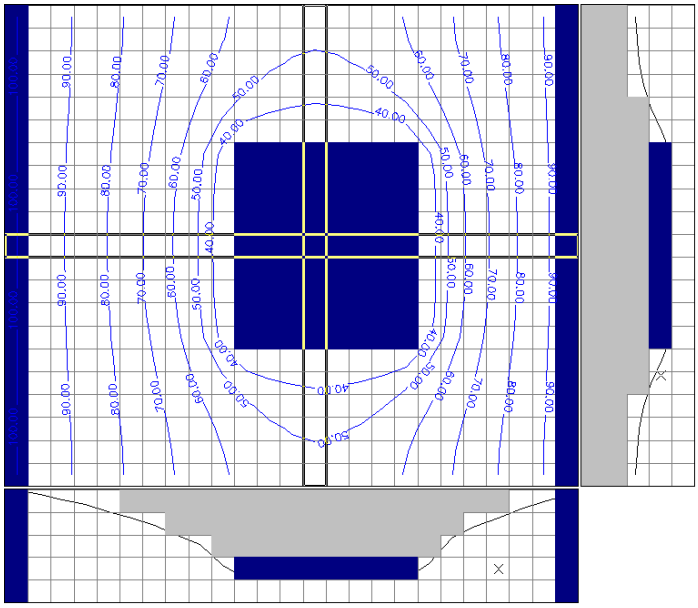


Fig. 5.20. Steady-state hydraulic head contours in layer 4

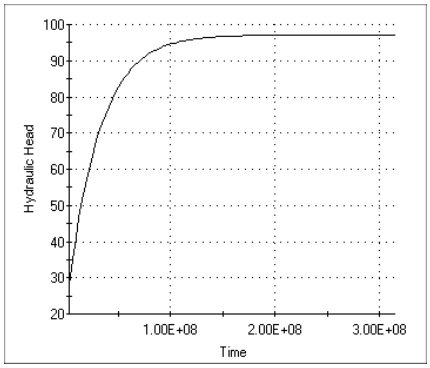


Fig. 5.21. Time-series curve of the water stage in the lake

5.2 EPA Instructional Problems

Folder: *pmdir*\examples\EPA Instructional Problems\

Overview of the Problem

The manual of instructional problems for MODFLOW (Andersen [5]) is intended to allow the student to have hands-on experience with the practical application of models. Twenty documented problems, complete with problem statements, input data sets, and discussion of results are presented in that manual. The problems are designed to cover modeling principles, specifics of input/output options available to the modeler, rules of thumb, and common modeling mistakes. You can find an electronic version of this manual in the folder \Document\Instructional Problems for MODFLOW (EPA) on the companion CD-ROM.

Modeling Approach and Simulation Results

Most of the models described in the manual of instructional problems have been rebuilt by using **PM**. You can find the models in sub-folders under path\examples\EPA Instructional Problems\. Although these models are ready-to-run, it is suggested to construct the models by yourself, because you will learn more through exercises and mistakes.

5.3 Parameter Estimation and Pumping Test

5.3.1 Basic Parameter Estimation Skill

Folder: *pmdir*\examples\calibration\calibration1

Overview of the Problem

Groundwater models are usually applied to conceptualize and understand a hydrologic system or to predict the outcome of a future change to the system. In order to provide some assurance that the model reflects the behavior or appearance of the flow system, it must be calibrated prior to use as a predictive tool. Model Calibration is accomplished by finding a set of model parameters, boundary conditions, and excitations or stresses that produce simulated heads (or drawdowns) and fluxes that match measurement values within an acceptable range of error. Model calibration can be performed by the hand-operated trial-and-error adjustment of aquifer parameters or by inverse models such as PEST, MODINV [32], MODFLOW/P [61], or MODFLOW-2000 [56] [63]. This example provides an exercise in model calibration with PEST. Specific details of this example are from Andersen [5].

Fig. 5.22 shows the idealized flow system and locations of observation boreholes. The flow system is a small, confined aquifer, which is strongly controlled by the river flowing across it. The aquifer is approximately 100 ft thick and is composed primarily of silty sand. The river is not in direct hydraulic connection with the aquifer, but acts as a leaky boundary condition, which can gain or lose water to the aquifer. Stage data for the river and riverbed elevation are listed in Table 5.2. Other boundary conditions are no-flow, which surround the square and define the areal extent of the aquifer.

Given constraints of uniform transmissivity and recharge, and additional data below, the task is to obtain a steady state calibration based on the measurements listed in Table 5.3.

Initial hydraulic head =	100.0 ft
Grid size =	15×15
Δx = Δy =	500 ft
River base flow at western model boundary =	10 cfs
River base flow at eastern model boundary =	11.125 cfs
Riverbed conductance =	0.01 ft^2/s

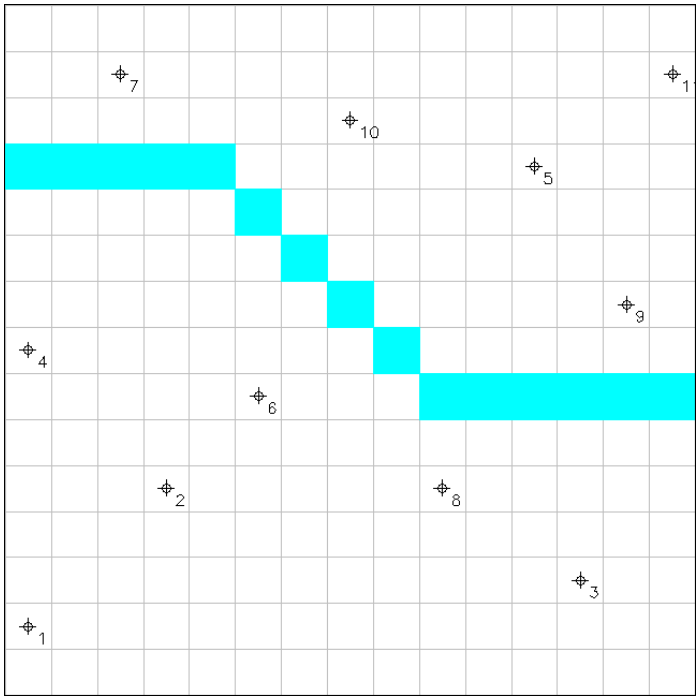


Fig. 5.22. Configuration of the aquifer system

Table 5.2 River data

Row	Column	Stage (ft)	Riverbed Elevation (ft)
4	1	100.0	90.0
4	2	100.0	90.0
4	3	100.0	90.0
4	4	99.0	89.0
4	5	99.0	89.0
5	6	98.0	88.0
6	7	97.0	86.0
7	8	96.0	86.0
8	9	95.0	85.0
9	10	94.0	84.0
9	11	94.0	84.0
9	12	94.0	84.0
9	13	94.0	84.0
9	14	93.0	83.0
9	15	93.0	83.0

Table 5.3 Measurement data

Borehole	X	Y	Head (ft)	Borehole	X	Y	Head (ft)
1	250	750	124.0	7	4750	2250	108.5
2	1750	2250	119.9	8	4750	2250	111.7
3	6250	1250	113.9	9	6750	4250	107.6
4	250	3750	116.1	10	3750	6250	111.3
5	5750	5750	113.0	11	7250	6750	115.6
6	2750	3250	114.0				

Modeling Approach and Simulation Results

The aquifer is simulated using a grid of one layer, 15 columns and 15 rows. A regular grid spacing 500 ft is used for each column and row. The layer type is 0:confined and the Transmissivity flag in the Layer Property dialog box is user-specified. Transmissivity and recharge are defined as estimated parameters (Note that the names of these two parameters are t_1 and rch_2).

The optimized parameter values and the correlation coefficient matrix calculated by PEST are listed below.

```
Parameter        Estimated         95% percent confidence limits
                 value             lower limit       upper limit
 t_1            1.000282E-02       9.902461E-03      1.010419E-02
 rch_2          1.996080E-08       1.983990E-08      2.008169E-08

Note: confidence limits provide only an indication of parameter uncertainty.
      They rely on a linearity assumption which  may not extend as far in
      parameter space as the confidence limits themselves - see PEST manual.

Parameter correlation coefficient matrix ----->

                  t_1          rch_2
t_1              1.000        0.9870
rch_2           0.9870         1.000
```

The diagonal elements of the correlation coefficient matrix are always unity. The off-diagonal elements are always between 1 and -1. The closer an off-diagonal element is to 1 or -1, the more highly correlated are the parameters corresponding to the row and column numbers of that element. For this example, transmissivity (parameter t_1) and recharge (parameter rch_2) are highly correlated, as is indicated by the value 0.987 of the correlation coefficient matrix. This means that these parameters are determined with a high degree of uncertainty in the parameter estimation process. A sensitivity analysis could be used to quantify the uncertainty in the calibrated model caused by uncertainty in the estimates of the aquifer parameters.

For our example, the only discharge is to the river and the only source is recharge. To be in steady state, these two must balance. Recharge must therefore be equal to 1.125 cfs (the river gain equals 11.125 cfs - 10 cfs). Spreading over the modeled area:

$$RECHARGE = \frac{1.125\ ft^3/s}{(15 \times 15) \times (500\ ft \times 500\ ft)} = 2 \times 10^{-8} ft/s \qquad (5.1)$$

The estimated parameter values are acceptable. A better procedure would have been to compute the recharge right away from Equation 5.1 and estimate only transmissivity.

5.3.2 Estimation of Pumping Rates

Folder: *pmdir*\examples\calibration\calibration2

Overview of the Problem

This example involves the encapsulation of a highly contaminated area. The aquifer in which the contaminated area is buried is unconfined, isotropic and of infinite areal extent. The extent of the contamination area is about $65\ m \times 65\ m$. The hydraulic head in the center of this area is about $9.45\ m$. The elevation of the aquifer top is $10\ m$ and the aquifer bottom is at $0\ m$. The hydraulic conductivity is uniformly $3 \times 10^{-4}\ m/s$. The unconfined storage coefficient (specific yield) is 0.2. Recharge is assumed to be zero. The groundwater flow is directed from west to east with a hydraulic gradient of 0.05 %.

To prevent contaminated water flow out of the area, a remedial measure is required. Different types and combinations of measures can be introduced for this purpose including a cutoff wall around the area, drains, and pumping wells. All measures are directed towards the same goal - a reduction of the hydraulic head in the contaminated area itself such that groundwater flows towards the contaminated area. To achieve this objective, a cutoff wall around this area and four pumping wells have been chosen. The cutoff wall is $0.5\ m$ thick and the hydraulic conductivity of the material is $5 \times 10^{-8}\ m/s$.

The task is to estimate the required pumping rate of the wells such that the steady-state piezometric head in the center of the contaminated area is $8\ m$. Furthermore, the duration until the steady state is reached should be calculated.

Modeling Approach and Simulation Results

The condition is simulated using a grid of one layer, 31 columns, and 31 rows. The layer type is 1:unconfined. Fig. 5.23 shows the model grid and the selected boundary conditions. The extent of the model is fairly large to ensure that the changes in hydraulic heads at the boundaries are not affected by the remedial measure. To obtain the hydraulic gradient of 0.05 %, the west and east sides of the model are assumed to be fixed-head boundaries with hydraulic head values of 9.8925 m and 9 m, respectively. The steady-state condition is simulated using one stress period and one time step. Although the length of the stress period is not relevant for a steady-state solution, we set the length to 1 so the computed head values can be compared with observed values. For this example, an "observation" borehole is set at the center of the contaminated area. The "observed" head at time 1 is set at $8\ m$ (the objective) using the Head Observation dialog box (see Section 2.6.1.14).

The configuration of the remedial measures is shown in Fig. 5.24. The pumping rates of the wells are defined as an estimated parameter by assigning the parameter number 1 to all four wells. Using PEST, the pumping rate of each well is estimated at about $7.9 \times 10^{-5}\ m^3/s$.

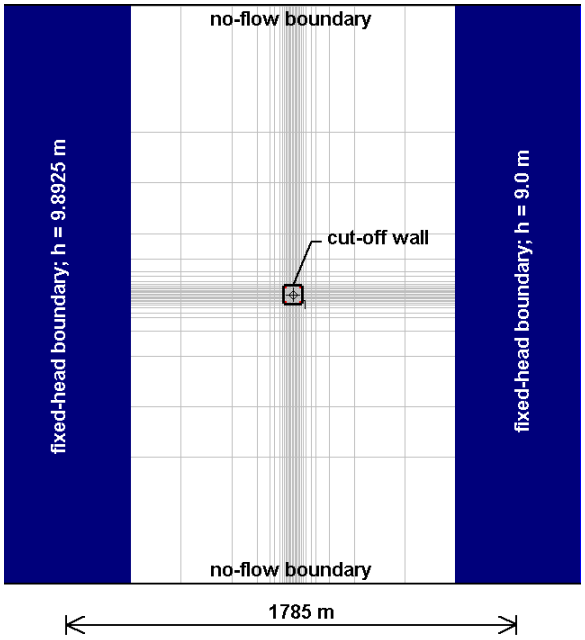


Fig. 5.23. Plan view of the model

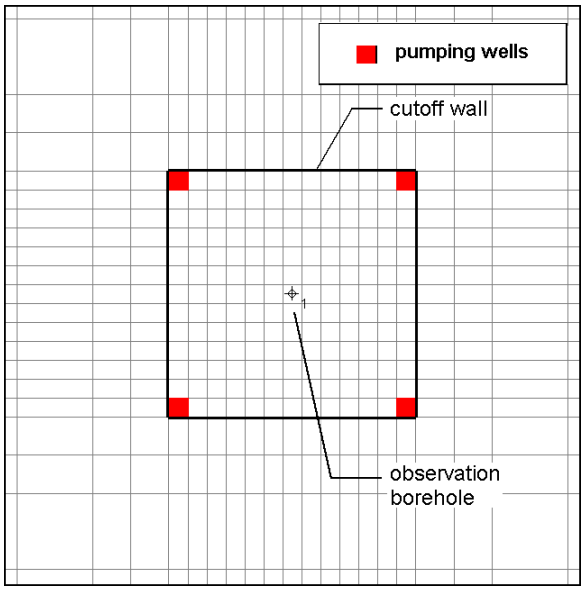


Fig. 5.24. Location of the cutoff wall and pumping wells

To calculate the required time to reach the steady-state condition, the estimated pumping rate of $7.9 \times 10^{-5}\ m^3/s$ is specified to each well. A transient simulation with one stress period (subdivided into 25 equal time steps) is carried out. The total simulation time is set at 1×10^8 seconds. The calculated head-time curve (Fig. 5.25) shows that the steady state is reached at $t \simeq 4 \times 10^7\ s$.

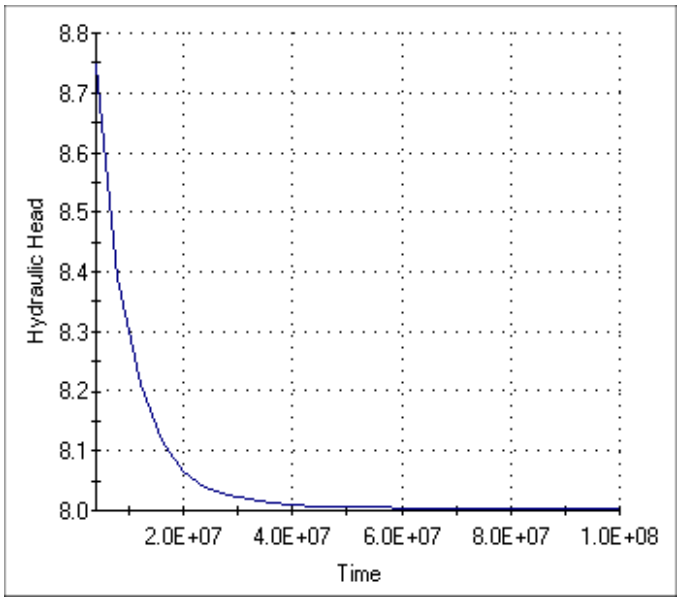


Fig. 5.25. Time series curve of the calculated hydraulic head at the center of the contaminated area

5.3.3 The Theis Solution – Transient Flow to a Well in a Confined Aquifer

Folder: *pmdir*\examples\calibration\calibration3

Overview of the Problem

This example gives an approximation of the Theis solution with a numerical model. Given the aquifer properties, transmissivity and confined storage coefficient, the Theis solution predicts drawdown in a confined aquifer at any distance from a well at any time since the start of pumping. The assumptions inherent in the Theis solution include:

1. The aquifer is homogeneous, isotropic and of uniform thickness,
2. The aquifer is confined between impermeable formations on top and bottom, and of infinite areal extent.
3. The initial piezometric surface is horizontal and uniform.
4. The pumping rate of the well is constant with time.
5. The well penetrates the entire aquifer and the well diameter is small.
6. Water is removed from storage instantaneously with decline in head.

A numerical model can represent all of these assumptions, with the exception of infinite areal extent.

In this example, a fully penetrating well is located at the center of the model domain and withdraws water at a constant rate. The drawdown of the hydraulic head is monitored with time at a borehole 55 m from the pumping well.

The task is to construct a numerical model, calculate the drawdown curve at the borehole, and compare it with the analytical (Theis) solution. The model parameters are given below.

Initial hydraulic head =	$0.0\ m$
Transmissivity =	$0.0023\ m^2/s$
Storage coefficient =	0.00075
Pumping rate =	$4 \times 10^{-3}\ m^3/s$
Total simulation time =	$86400\ s$
Number of time steps =	20
Time step multiplier =	1.3
Number of SIP iteration parameters =	5
Convergence criterion of head change =	$0.0001\ m$
Maximum number of iterations =	50

Modeling Approach and Simulation Results

To meet the requirement of an infinite areal extent, the modeled domain is chosen fairly large (The boundary could alternatively be moved even further from the pumping well by using the General Head Boundary, see Section 5.1.2). A single layer model simulates the aquifer. An increasing grid spacing expansion is used to extend the model boundaries (Fig. 5.26). The layer type is 0:confined. In the Layer Property dialog box, the flags of Transmissivity and Storage Coefficient are set to *User-specified*. The top and bottom elevations of the model layer are not required in this example since the geometrical information is included in Transmissivity and Storage Coefficient.

The analytical drawdown values at the borehole are specified in the Drawdown Observation dialog box (*Models* | *Modflow* | *Drawdown Observation*. Both the analytical and calculated drawdown curves are shown in Fig. 5.27. An exact comparison is not attained because of the approximations made in the numerical model. These include: (1) use of a discrete rather than continuous spatial domain, (2) use of a discrete rather than continuous time domain, (3) use of an iterative solution with a convergence tolerance, (4) artificial placement of boundaries.

In practice, we can use this model to estimate transmissivity and confined storage coefficient by specifying the real observation time and data in the Drawdown Observation dialog box. By defining transmissivity and storage coefficient as estimated parameters, the parameter estimation program PEST can estimate the parameters automatically. Select *Models* | *PEST (Parameter Estimation)* | *Run* to see how

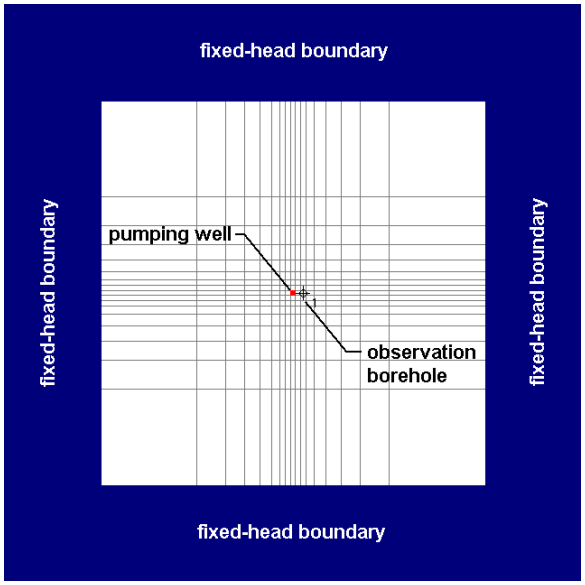


Fig. 5.26. Plan view of the model

the parameter estimation programs work. Since the analytical drawdown values were used as the observations, the results from the parameter estimation programs must be transmissivity = $0.0023\ m^2/s$ and storage coefficient = 0.00075.

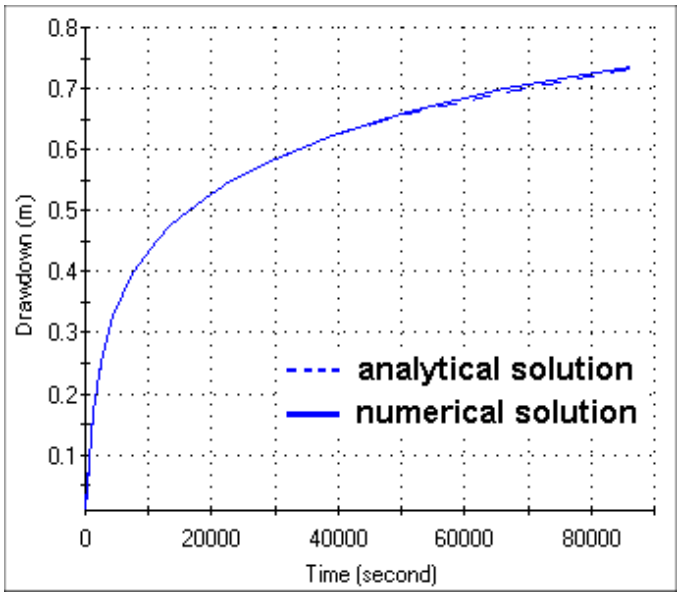


Fig. 5.27. Time-series curves of the calculated and observed drawdown values

5.3.4 The Hantush and Jacob Solution – Transient Flow to a Well in a Leaky Confined Aquifer

Folder: *pmdir*\examples\calibration\calibration4

Overview of the Problem

This example demonstrates how to approach leaky confined aquifers. A leaky confined aquifer is overlaid and/or underlaid by geologic formations, which are not completely impermeable and can transmit water at a sufficient rate (Fig. 5.28). Hantush and Jacob [52] give an analytical solution to describe the drawdown with time during pumping with a well in a leaky confined aquifer. In addition to the assumptions in the Theis solution, the analytical solution requires two assumptions – the hydraulic head in the overlying or underlying aquifer is constant during pumping in the leaky confined aquifer and the rate of leakage into the pumped aquifer is proportional to drawdown.

In this example, a pumping well withdraws water at a constant rate from the leaky confined aquifer. The drawdown of the hydraulic head is monitored with time at a borehole 55 m from the pumping well. The borehole is located in the leaky confined aquifer. The initial hydraulic head is 8 m everywhere. Specific yield and effective porosity are 0.1. The other aquifer parameters are given in Fig. 5.28. The analytical solution for this case is given in Table 5.4.

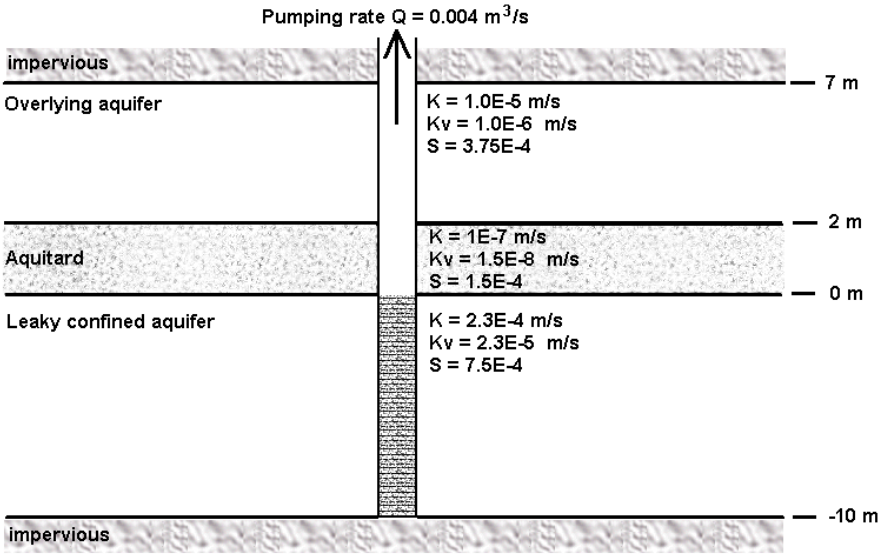


Fig. 5.28. Configuration of the leaky aquifer system and the aquifer parameters

The task is to construct a numerical model, calculate the drawdown curve at the borehole and compare it with the Hantush-Jacob solution. Note that the parameters for the confined leaky aquifer are the same as in the previous example, so we can compare the results of these two examples.

Modeling Approach and Simulation Results

The modeled domain is the same as in the previous example. Three model layers are used to simulate the system. The layer type of all three layers is 3:confined/unconfined (transmissivity varies). In the Layer Property dialog box, the Storage Coefficient flag is set to user-specified and the Transmissivity flag is calculated. All model cells in the first model layer are fixed-head cells and all other cells are specified as active cells. A transient flow simulation is performed for a stress period with the length of 49320 seconds, 20 time steps and a time-step multiplier of 1.3. For comparison, the analytical solution is entered in the Drawdown Observation dialog box. Fig. 5.29 shows the numerical and analytical drawdown-time curves at the observation borehole, which is at a distance of 55 m from the pumping well. The match of these two curves is very good.

While the use of the analytical solution is limited to the primary assumptions, the numerical model can be used to evaluate pumping tests, even if the confining aquitard (Fig. 5.28) has a higher value of the vertical hydraulic conductivity and the hydraulic head in the overlying aquifer is not constant during the pumping. To do this, simply specify all model cells as active cells. This is allowed because the simulation time is normally very short and the extent of the model domain is relative large, so that at the end of a transient flow simulation the drawdown values at the model boundaries are acceptable low.

If the vertical hydraulic conductivity of the aquitard is known, we can use PEST to estimate the horizontal hydraulic conductivity and storage coefficient of the leaky aquifer by defining them as estimated parameters. Click *Models* | *PEST* | *Run* to see how the parameter estimation programs work. Because the analytical drawdown values were used as the observations, the results from the parameter estimation programs must be horizontal hydraulic conductivity = $2.3 \times 10^{-4}\ m/s$ and storage coefficient = 0.00075. If the vertical hydraulic conductivity is unknown and needs

Table 5.4 Analytical solution for the drawdown with time

Time (seconds)	Drawdown (m)	Time (seconds)	Drawdown (m)
123	0.0067	4932	0.336
247	0.03	12330	0.449
352	0.052	24660	0.529
493	0.077	35228	0.564
1233	0.168	49320	0.595
2466	0.25	123300	0.652
3523	0.294		

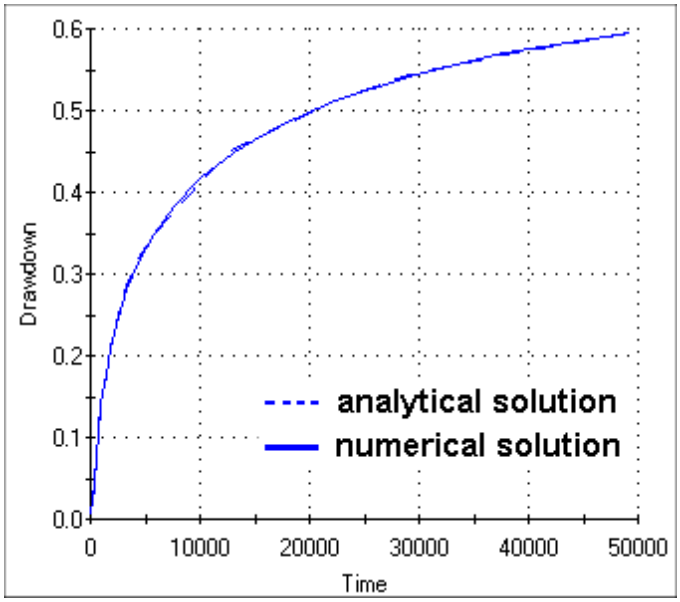


Fig. 5.29. Configuration of the leaky aquifer system and the aquifer parameters

to be estimated, we will need additional drawdown values in the overlying aquifer during the pumping test.

5.3.5 Parameter Estimation with MODFLOW-2000: Test Case 1

Folder: *pmdir*\examples\calibration\calibration5\

Overview of the Problem

This example model is adapted from Hill and others [63]. The physical system for this example is shown in Fig. 5.30. The synthetic system consists of two confined aquifers separated by a confining unit. Each aquifer is 50 m thick, and the confining unit is 10 m thick. The river is hydraulically connected to aquifer 1. Groundwater flow from the hillside adjoining the system is connected to aquifers 1 and 2 at the boundary farthest from the river.

The parameters that define aquifer properties are shown in Fig. 5.30 and listed in Table 5.5. The observations of head and river-flow gain used in the parameter estimation were generated by running the model with the given parameter values and the parameter multiplier PARVAL = 1 for all parameters (the actual parameter values used in the simulation are calculated as the product of the parameter values and the parameter multiplier PARVAL). Different starting values are used for PARVAL and the estimated PARVAL values are expected to be close to 1.

The hydraulic conductivity of the second aquifer is known to increase with distance from the river. The variation is defined by a step function with the value 1.0 $\times$ HK_3 in columns 1 and 2, 2.0 $\times$ HK_3 in columns 3 and 4, and so on to the value 9.0 $\times$ HK_3 in columns 17 and 18.

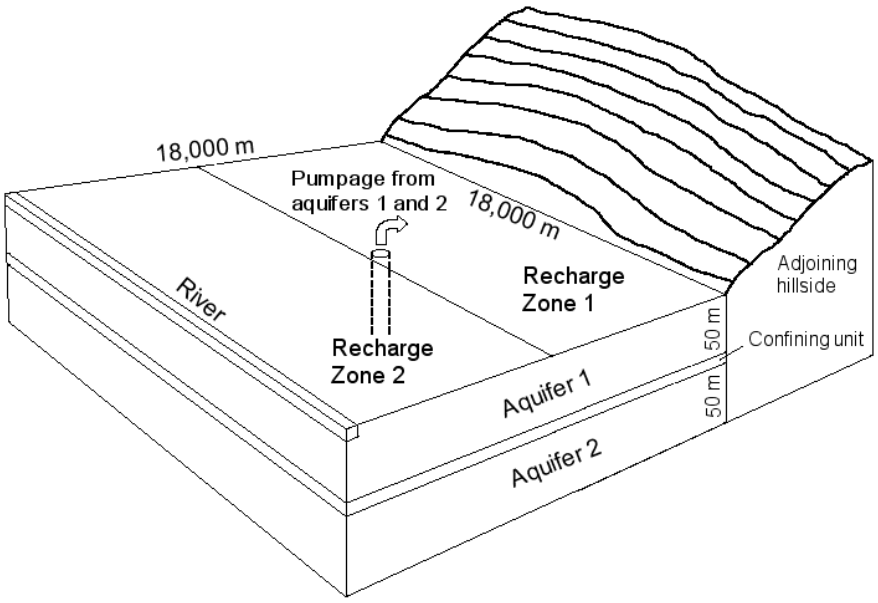


Fig. 5.30. Physical system for test case 1. Adapted from Hill and others [63]

Stresses on the system include (1) areal recharge to aquifer 1 in the area near the stream (zone 1) and in the area farther from the stream (zone 2), and (2) groundwater abstraction from wells in each of the two layers. The pumping rates from aquifers 1 and 2 are assumed to be the same.

Modeling Approach and Simulation Results

For the finite-difference method, the system is discretized into square 1,000 m by 1,000 m cells, so that the grid has 18 rows and 18 columns. Three model layers are used. Layers 1 and 3 represent aquifers 1 and 2, respectively. Layer 2 represents the confining unit. A fairly small value of $1 \times 10^{-9}\ m/s$ is assigned to horizontal hydraulic conductivity of layer 2 so that the groundwater flows vertically through the confining unit.

Time discretization for the model run is specified to simulate a period of steady-state conditions with no pumping followed by a transient-state period with a constant rate of pumping. The steady-state period is simulated with one stress period having one time step. The transient period is simulated with four stress periods: the first three are 87162, 261486, and 522972 seconds long, and each has one time step; the fourth is 2.356745×10^7 seconds long and has 9 time steps, and each time-step length is 1.2 times the length of the previous time-step length.

Ground-water flow into the system from the adjoining hillside is represented using the General-Head Boundary Package. Thirty-six general-head-boundary cells are specified in column 18 of layers 1 and 3, each having an external head of 350 m and a hydraulic conductance of $1 \times 10^{-7}\ m^2/s$.

The river is treated as a head-dependent boundary, which is simulated using the River Package to designate 18 river cells in column 1 of layer 1; the head in the river is 100 m. The parameter RIV_1 specifies the conductance of the riverbed for each cell.

Recharge in zone 1 (RCH_1) applies to cells in columns 1 through 9; recharge in zone 2 (RCH_2) applies to cells in columns 10 through 18. The pumpage is simulated using the Well Package. Wells are located at the center of the cells at row 9, column 10; there is one well is in each of layer 1 and 3. Both wells have the same pumping rate. The parameter WEL_1 specifies the pumping rate for each of the wells.

As shown in Table 5.5, the estimated values of PARVAL are, as expected, close to 1. The final parameter values are obtained by multiplying the estimated PARVAL with the parameter's initial cell-values.

Table 5.5 Parameters defined for MODFLOW-2000 test case 1, parameter values, starting and estimated PARVAL

PARNAM	**Description**	**Parameter values**	**Starting PARVAL**	**Estimated PARVAL**
HK_1	Hydraulic conductivity of layer1	$4 \times 10^{-4}\ [m/s]$	0.75	1.00000
HK_3	Hydraulic conductivity of layer 3 under the river	$4.4 \times 10^{-5}\ [m/s]$	0.9	1.00013
RCH_1	Recharge rate in zone 1	$1 \times 10^{-8}\ [m/s]$	2.0	0.99997
RCH_2	Recharge rate in zone 2	$1.5 \times 10^{-8}\ [m/s]$	0.66	1.00005
RIV_1	Hydraulic conductance of the riverbed	$1.2\ [m^2/s]$	1.2	1.00036
SS_1	Specific storage of layer 1	$4 \times 10^{-5}\ [1/m]$	0.65	1.00006
SS_3	Specific storage of layer 3	$2 \times 10^{-6}\ [1/m]$	2.0	0.999274
WEL_1	Pumping rate in each of layers 1 and 3	$-1.0\ [m^3/s]$	1.1	1.00003
VK_2	Vertical hydraulic conductivity of layer 2	$2 \times 10^{-7}\ [m/s]$	0.50	1.00017

5.3.6 Parameter Estimation with MODFLOW-2000: Test Case 2

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Overview of the Problem

This example model is adapted from Hill and others [63]. The model grid shown in Fig. 5.31 has a uniform grid spacing of 1500 m in the horizontal and has 247 active cells in each of three layers. Layers 1, 2, and 3 have a constant thickness of 500 m, 750 m, and 1500 m, respectively. Hydraulic conductivity is divided into four zones, each of which is present in the middle layer and three of which are present in the top and bottom layers. Constant-head boundaries comprise portions of the western and eastern boundaries, with no flow across the remaining boundaries. Head-dependent boundaries representing springs are simulated using both the Drain and General-Head Boundary Packages. Wells are present at selected cells, with pumpage at rates ranging from 100 to 200 m^3/d.

Modeling Approach and Simulation Results

Ten parameters were identified for inclusion in the parameter estimation and are described in Table 5.6 along with their true (assigned) values. The observations used in the parameter estimation were generated by running the model with the true parameter values and the parameter multiplier PARVAL = 1 for all parameters (the actual parameter values used in the simulation are calculated as the product of the parameter values and the parameter multiplier PARVAL). The locations of the 42 "observed" hydraulic heads are shown in Fig. 5.31. The flows simulated at the head-dependent boundaries also were used as observations for the parameter estimation. In this ideal situation, the estimated values of the parameter multiplier PARVAL are expected to be close to 1. If this is accomplished, it suggests that the observation sensitivities are calculated correctly and that the regression is performing correctly.

The final parameter values are obtained by multiplying the estimated PARVAL with the parameter's initial values.

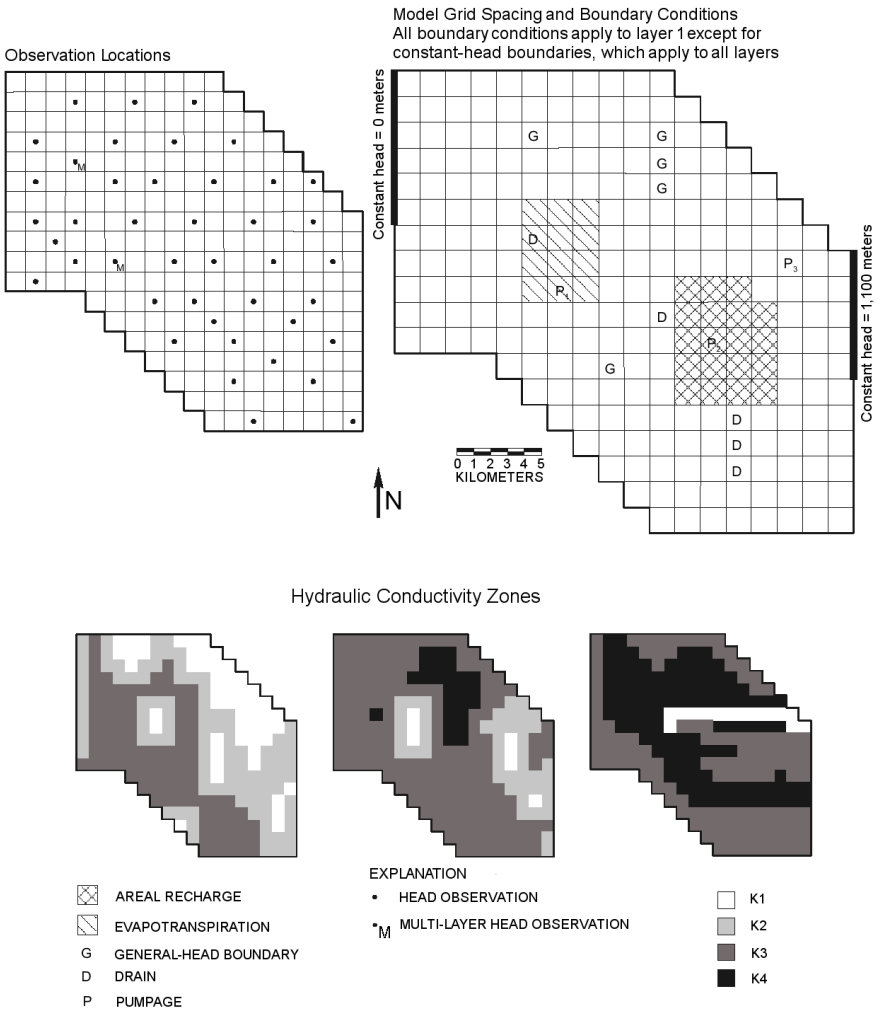

Fig. 5.31. Test case 2 model grid, boundary conditions, observation locations and hydraulic conductivity zonation used in parameter estimation. Adapted from Hill and others [63]

Table 5.6 Parameters defined for MODFLOW-2000 test case 2, parameter values, starting and estimated PARVAL

PARNAM	**Description**	**Parameter values**	**Starting PARVAL**	**Estimated PARVAL**
HK_1	Hydraulic conductivity of zone 1 (see Fig. 5.31)	$1.0\ [m/d]$	1.5	0.999990
HK_2	Hydraulic conductivity of zone 2 (see Fig. 5.31)	$0.01\ [m/d]$	0.5	0.999989
HK_3	Hydraulic conductivity of zone 3 (see Fig. 5.31)	$1 \times 10^{-4}\ [m/d]$	1.2	0.999987
HK_4	Hydraulic conductivity of zone 4 (see Fig. 5.31)	$1 \times 10^{-6}\ [m/d]$	2.0	1.000330
VANI_12	Vertical anisotropy of layers 1 and 2	4	0.25	1.000010
VANI_3	Vertical anisotropy of layer 3	1	10.0	1.000040
RCH_1	Areal recharge rate applied to the area shown in Fig. 5.31	$3.1 \times 10^{-4}\ [m/d]$	1.42	0.999988
EVT_1	Maximum evapotranspiration rate applied to area shown in Fig. 5.31	$4 \times 10^{-4}\ [m/d]$	0.75	0.999968
GHB_1	Conductance of head-dependent boundaries represented using the General-Head Boundary package (G in Fig. 5.31)	$1.0\ [m^2/d]$	0.5	0.999988
DRN_1	Conductance of head-dependent boundaries represented using the Drain package (D in Fig. 5.31)	$1.0\ [m^2/d]$	2.0	0.999990

5.4 Geotechnical Problems

5.4.1 Inflow of Water into an Excavation Pit

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Overview of the Problem

This example is adapted from Kinzelbach and Rausch [72]. Fig. 5.32 shows the plan view and a cross section through a shallow aquifer situated in a valley. In the north the aquifer is bounded by the outcrop of the sediments in the valley, while the south boundary is a river, which is in contact with the aquifer. The aquifer extends several kilometers to the west and east; it is unconfined, homogeneous and isotropic. The top and bottom elevations of the aquifer are $7\ m$ and $0\ m$, respectively. The average horizontal hydraulic conductivity of the sandy sediments is $0.001\ m/s$; the effective porosity is 0.15. The groundwater recharge from precipitation is $6 \times 10^{-9}\ m^3/s/m^2$. The water stage in the river is $5\ m$ above the flat aquifer bottom, which is the reference level for the simulation. At a distance of $200\ m$ from the river there is an excavation pit. The length of the pit is $200\ m$, the width $100\ m$. The bottom of the excavation is $3\ m$ above the aquifer bottom.

The task is to calculate the inflow into the pit and show head contours and catchment area of the pit.

Modeling Approach and Simulation Results

The aquifer is simulated using a grid of one layer, 40 columns and 19 rows. A regular grid spacing of $50\ m$ is used for each column and row. The layer type is 1:unconfined. To simplify the simulation, use of symmetry is made by modeling only half the domain. The river and the pit are modeled as fixed-head boundaries with hydraulic heads of h = $5\ m$ and $3\ m$, respectively. All other boundaries are no-flow boundaries. The distance between the eastern no-flow boundary and the pit is not known a priori and must be selected large enough so that the pit does not influence it. Whether the choice was adequate can be easily checked by increasing the sizes of the last few columns and calculating again. If the results do not change appreciably the first computation was fine. Fig. 5.33 shows the head contours, the catchment area of the excavation and two cross-sections. Using the Water budget calculator, the inflow into the pit is calculated at $2 \times 0.0129\ m^3/s = 0.0258\ m^3/s$.

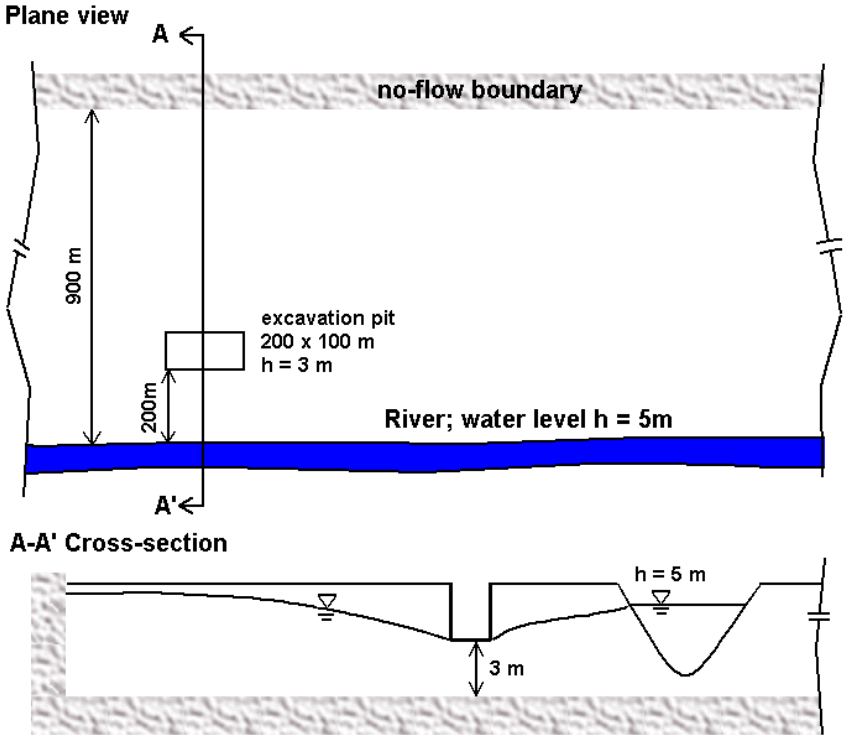

Fig. 5.32. Configuration of the physical system

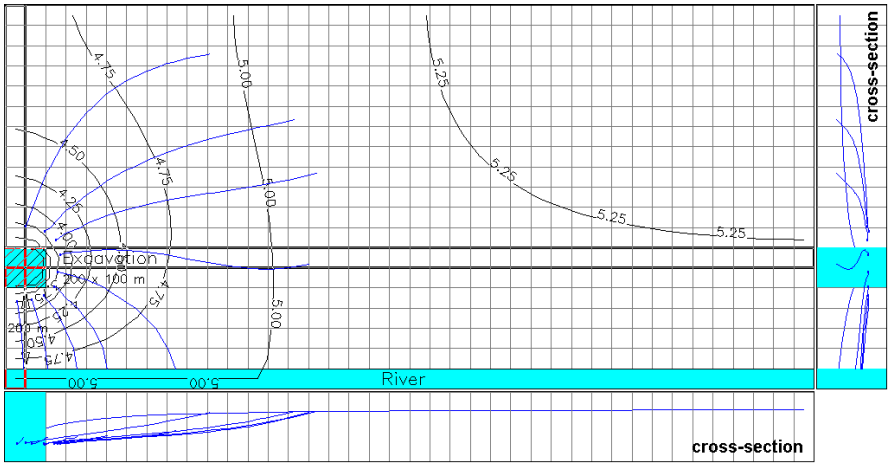

Fig. 5.33. Simulated head distribution and catchment area of the excavation pit

5.4.2 Flow Net and Seepage under a Weir

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Overview of the Problem

This example is adapted from Kinzelbach and Rausch [72]. An impervious weir is partially embedded in a confined aquifer. The aquifer is assumed to be homogeneous with a hydraulic conductivity of the aquifer of $0.0005\ m/s$ and a thickness of $9\ m$. The effective porosity of the aquifer is 0.15. The boundary conditions are shown in Fig. 5.34. Calculate the flow net and the flux through the aquifer for the cases that (1) the aquifer is isotropic and (2) the aquifer is anisotropic with an anisotropy factor of 0.2.

Modeling Approach and Simulation Results

To compute the head distribution and the corresponding flowlines it is sufficient to consider a vertical cross-section of the aquifer with a uniform thickness of $1\ m$. In this example, the vertical cross-section is represented by a model with a grid of one layer, 65 columns and 9 rows. A regular grid spacing of 1 m is used for each column and row. The layer type is 0:confined. Fig. 5.35 shows the cross section, the selected model grid and the boundary conditions. The boundaries at the upstream and downstream of the weir are modeled as fixed-head boundaries with h = $12\ m$ and h = $10\ m$ above reference level, respectively. The aquifer bottom and the weir itself are modeled as no-flow boundaries.

Fig. 5.36 shows the flow net for the isotropic case. The head values range from 10 to $12\ m$ with a head increment of 0.1 m. The flux through the aquifer (per meter width of the weir) is $3.65 \times 10^{-4}\ m^3/s/m$ ($\simeq 31.56\ m^3/day/m$). Fig. 5.37 shows the flow net for the aquifer in the anisotropic case. The flux through the aquifer is now only $2.5 \times 10^{-4}\ m^3/s/m$ ($\simeq 21.6\ m^3/day/m$). Note that in a homogeneous and anisotropic medium, flowlines intersect head contours at right angle only where flow is parallel to one of the principal directions of hydraulic conductivity.

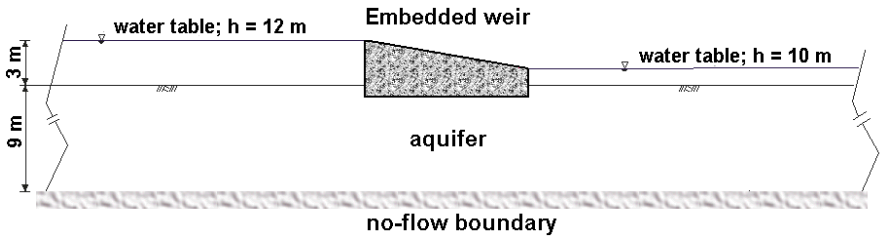

Fig. 5.34. Configuration of the physical system

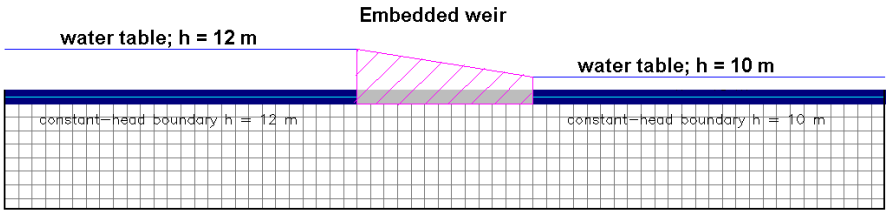

Fig. 5.35. Model grid and the boundary conditions

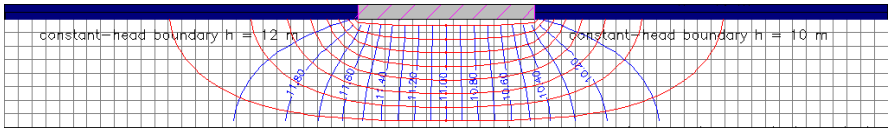

Fig. 5.36. Flowlines and calculated head contours for isotropic medium

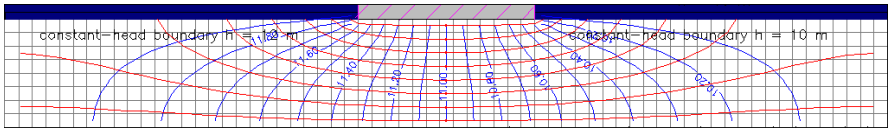

Fig. 5.37. Flowlines and calculated head contours for anisotropic medium

5.4.3 Seepage Surface through a Dam

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Overview of the Problem

This example is adapted from Kinzelbach and Rausch [72]. It demonstrates how to calculate the seepage surface using a vertical cross-sectional model. As shown in Fig. 5.38, the length of the dam is 100 m; the thickness and height are 10 m. The water table is 10 m at the upstream side of the dam and 2 m at the downstream side. The material of the dam is homogeneous and isotropic with a hydraulic conductivity of $1 \times 10^{-5}\ m/s$. The unrealistic bank slope is used here to simplify the data input.

The task is to calculate the seepage surface and the seepage rate by using a vertical cross-sectional numerical model. Compare the seepage rate with an analytical solution after Dupuit.

Modeling Approach and Simulation Results

To compute the head distribution and the seepage surface, it is sufficient to consider a vertical cross-section of the aquifer with a uniform thickness of $1\ m$. The aquifer is simulated using a grid of one layer, 21 columns and 20 rows. A regular grid spacing of $0.5\ m$ is used for each column. The layer type is 0:confined. The boundary at the upstream side of the dam is modeled as fixed-head boundary with the hydraulic head h = $10\ m$. On the right-hand side of the dam, there are four fixed-head cells with h = $2\ m$. The other cells on this boundary are modeled as drain cells with a high drain hydraulic conductance [L^2T^{-1}] value. The elevation of the drain is set the same as the bottom elevation of each cell, for example the $2.0\ m$ for the cell [1, 16, 21] and $2.5\ m$ for the cell [1, 15, 21]. The drain cells are activated only if water table is higher than the level of the drain. The selected model grid and the boundary conditions are shown in Fig. 5.39. Except the four fixed-head cells at the right-hand side of the dam, the initial hydraulic head for all cells are $10\ m$.

The first step in solving this problem is to carry out a steady-state flow simulation with these data. Fig. 5.40 shows the calculated hydraulic heads. By comparing the calculated heads with the elevation of the cell bottom, we can easily find that the hydraulic heads of some of the cells at the upper-right corner of the model are lower than the cell bottom. This means that these cells went dry. In the second step, these dry cells will be defined as inactive cells by setting IBOUND = 0 and a steady-state flow simulation will be carried out again. Now, it is possible that some of the calculated heads are higher than the top elevation of the highest active cell. In this case, these cells will be defined as active and a steady-state flow simulation will be performed again. This iterative solution will be repeated until the water table remains unchanged between two iteration steps. Fig. 5.41 shows the calculated head distribution and the form of the seepage surface. The seepage rate is about $4.8 \times 10^{-5}\ m^3/s/m$ and the total seepage rate through the dam (length $100\ m$) is $4.8 \times 10^{-3}\ m^3/s$.

The analytical solution of the seepage rate after the Dupuit assumption is

$$Q = K \cdot B \cdot \frac{\left({h_1}^2 - {h_2}^2\right)}{2 \cdot L} = K \cdot \frac{h_1 + h_2}{2} \cdot B \cdot \frac{h_1 - h_2}{L} \tag{5.2}$$

where B is the length of the dam, L is the thickness of the dam, K is the hydraulic conductivity, h_1 and h_2 are the heads at the upstream and downstream sides of the dam, respectively. The modified form of the analytical solution is Darcy's Law with a mean transmissivity of $K \cdot (h1 + h2)/2$. For this example with h_1 = 10 m, h_2 = 2 m, L = 10 m, B = 100 m and $K = 1 \times 10^{-5}\ m/s$, the seepage rate Q is exactly equal to $4.8 \times 10^{-3}\ m^3/s$.

Note that in a 3D model such as MODFLOW this problem should be solved as a vertical cross-section by using the wetting capability (Section 2.6.1.12) with a discretization of 20 layers, 1 row, and 21 columns. It is, however, instructive to try out the iteration by hand, to better appreciate the wetting procedure. The attentive reader will notice that using the 2D horizontal model for a vertical cross-section is not quite correct. The transmissivity of a cell is not changed with the water table location. This corresponds to choosing the layer type 2: confined/unconfined (Transmissivity = const.) in a multi-layer MODFLOW model. However, the wetting capability cannot be used for layers of type 2, because model cells of this layer type do not convert between dry and wet. Therefore, layer type 3 should be used for all layers.

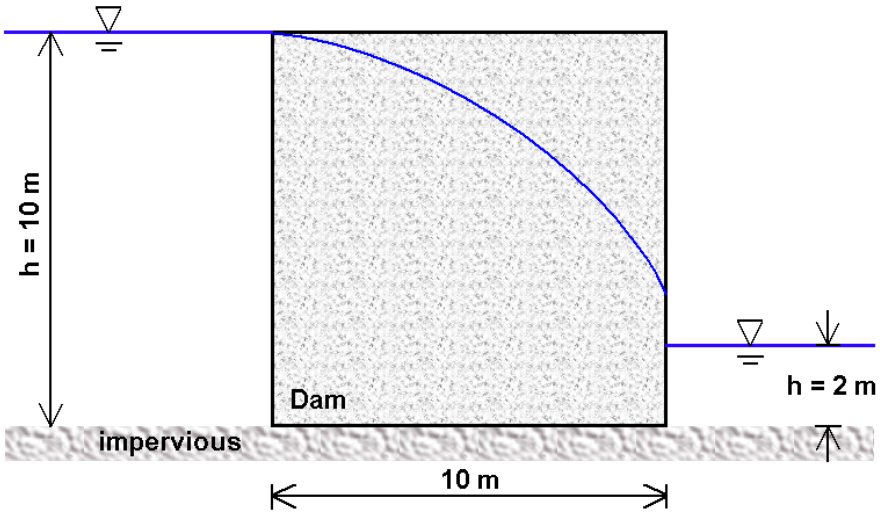


Fig. 5.38. Seepage surface through a dam

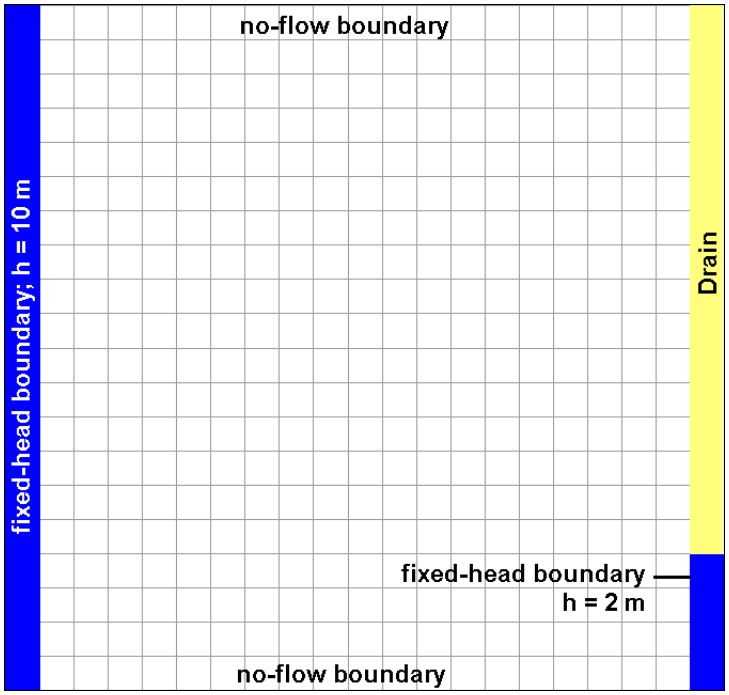


Fig. 5.39. Model grid and the boundary conditions

Cells in the J-direction

I \ J	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	elevation of the cell bottom [m]
1	10	9.75	9.50	9.25	9.01	8.77	8.54	8.31	8.08	7.86	7.66	7.46	7.27	7.10	6.94	6.80	6.68	6.58	6.51	6.46	6.43	9.5
2	10	9.75	9.50	9.25	9.01	8.77	8.53	8.30	8.07	7.86	7.65	7.45	7.26	7.08	6.92	6.78	6.66	6.56	6.48	6.43	6.40	9.0
3	10	9.74	9.50	9.25	9.00	8.76	8.52	8.29	8.06	7.84	7.63	7.42	7.23	7.05	6.89	6.74	6.62	6.51	6.43	6.38	6.35	8.5
4	10	9.74	9.49	9.24	8.99	8.75	8.51	8.27	8.04	7.81	7.60	7.39	7.19	7.01	6.84	6.69	6.55	6.44	6.36	6.30	6.27	8.0
5	10	9.74	9.49	9.23	8.98	8.73	8.49	8.24	8.01	7.78	7.56	7.34	7.14	6.95	6.77	6.61	6.47	6.35	6.26	6.19	6.16	7.5
6	10	9.74	9.48	9.22	8.97	8.71	8.46	8.22	7.97	7.74	7.51	7.29	7.07	6.87	6.68	6.51	6.36	6.23	6.13	6.05	6.02	7.0
7	10	9.73	9.47	9.21	8.95	8.69	8.44	8.18	7.93	7.69	7.45	7.22	7.00	6.78	6.58	6.40	6.23	6.08	5.96	5.88	5.83	6.5
8	10	9.73	9.46	9.20	8.93	8.67	8.40	8.15	7.89	7.64	7.39	7.15	6.91	6.68	6.46	6.26	6.07	5.91	5.77	5.67	5.61	6.0
9	10	9.72	9.45	9.18	8.91	8.64	8.37	8.11	7.84	7.58	7.32	7.06	6.81	6.57	6.33	6.11	5.90	5.70	5.54	5.41	5.33	5.5
10	10	9.72	9.44	9.16	8.89	8.61	8.34	8.06	7.79	7.52	7.25	6.98	6.71	6.45	6.19	5.94	5.70	5.48	5.27	5.09	4.97	5.0
11	10	9.71	9.43	9.15	8.87	8.58	8.30	8.02	7.74	7.46	7.17	6.89	6.61	6.33	6.05	5.77	5.50	5.23	4.97	4.72	4.50	4.5
12	10	9.71	9.42	9.13	8.85	8.56	8.27	7.98	7.69	7.39	7.10	6.80	6.50	6.20	5.90	5.59	5.28	4.97	4.65	4.33	4.00	4.0
13	10	9.70	9.41	9.12	8.82	8.53	8.23	7.94	7.63	7.33	7.03	6.71	6.40	6.08	5.75	5.42	5.08	4.72	4.35	3.94	3.50	3.5
14	10	9.70	9.40	9.10	8.81	8.50	8.20	7.90	7.59	7.27	6.96	6.63	6.30	5.96	5.61	5.25	4.88	4.49	4.07	3.60	3.00	3.0
15	10	9.69	9.39	9.09	8.79	8.48	8.17	7.86	7.54	7.22	6.89	6.56	6.21	5.86	5.49	5.10	4.70	4.28	3.84	3.39	3.00	2.5
16	10	9.69	9.39	9.08	8.77	8.46	8.15	7.83	7.50	7.17	6.84	6.49	6.13	5.76	5.38	4.97	4.54	4.09	3.62	3.13	2.71	2.0
17	10	9.69	9.38	9.07	8.76	8.44	8.13	7.8	7.47	7.14	6.79	6.43	6.07	5.68	5.28	4.86	4.41	3.93	3.40	2.80	2.0	1.5
18	10	9.69	9.37	9.06	8.75	8.43	8.11	7.78	7.45	7.11	6.75	6.39	6.02	5.62	5.21	4.78	4.31	3.81	3.27	2.67	2.0	1.0
19	10	9.68	9.37	9.06	8.74	8.42	8.10	7.77	7.43	7.09	6.73	6.36	5.98	5.58	5.16	4.72	4.25	3.74	3.20	2.61	2.0	0.5
20	10	9.68	9.37	9.06	8.74	8.42	8.09	7.76	7.42	7.07	6.72	6.35	5.96	5.56	5.14	4.69	4.21	3.71	3.17	2.59	2.0	0.0

Cells in the I-direction

Fig. 5.40. Calculated hydraulic heads after one iteration step

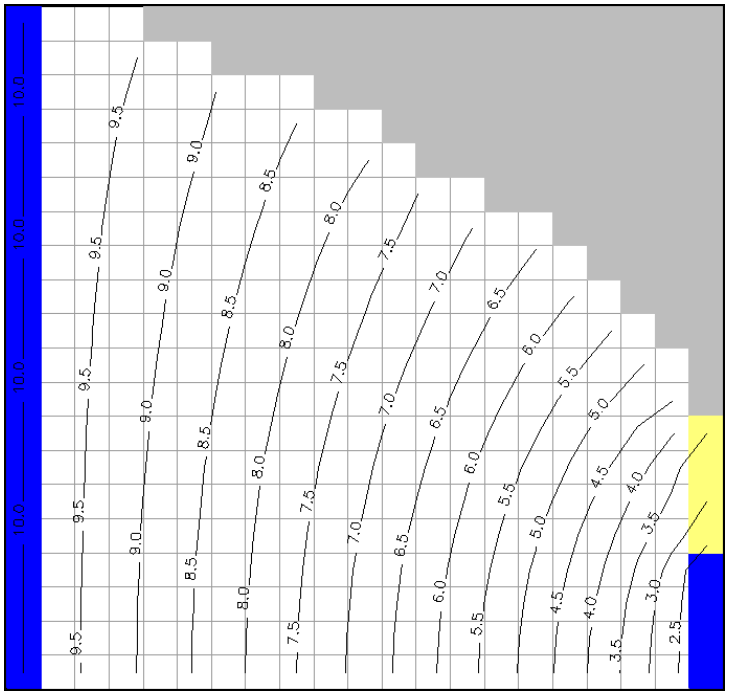


Fig. 5.41. Calculated hydraulic heads distribution and the form of the seepage surface

5.4.4 Cutoff Wall

Folder: *pmdir*\examples\geotechniques\geo4

Overview of the Problem

As shown in Fig. 5.42, a highly contaminated area is located in the first stratigraphic unit of an unconfined aquifer. To the west and east of the aquifer exist fixed-head boundaries with the hydraulic head h = -0.4 m and +0.5 m. The aquifer consists of five stratigraphic units. Each unit is horizontally isotropic with uniform thickness. The elevations and horizontal hydraulic conductivities are illustrated in Fig. 5.42. The vertical hydraulic conductivities are assumed to be a tenth of the horizontal hydraulic conductivities. The effective porosity of the aquifer is 0.15. The recharge rate is $1 \times 10^{-8}\ m/s$.

Because of the high cost, the contaminants cannot be removed. The task is to develop a strategy to isolate the contamination. There are four subtasks to be done.

1. Construct a groundwater flow model and perform a steady-state flow simulation by using the data given above and the model grid given in Fig. 5.42.
2. Geotechnical measures, such as cutoff wall, impervious cover, drain etc., can be considered as an alternative. Calculate flowlines for the case that a cutoff wall has been built to a depth of -8m and the recharge rate within the cutoff wall is reduced to zero by an impervious cover. The location of the cutoff wall is given in Fig. 5.42. When calculating the flowlines, particles should be started from the contaminated area.
3. Repeat previous step for the case that the cutoff wall reaches the depth -10m.
4. Use a pumping well located in the cell [row, column] = [12, 6] to capture the contaminants. Calculate the required pumping rate and penetration depth.

Modeling Approach and Simulation Results

The aquifer is simulated using a grid of 5 layers, 23 rows, and 23 columns. All layers have the same layer type 3: confined/unconfined (Transmissivity varies). The cutoff wall is modeled by using the Horizontal-Flow Barriers package. An impervious cover can be easily simulated by reducing the recharge rate. Figures 5.43 and 5.44 show the flowlines by performing forward and backward particle-tracking with PMPATH. The particles are initially placed in the center of each cell, which is located in the first model layer and within the cutoff wall. It is obvious that the contaminants will be "washed out", even if the cutoff wall is going deeper.

The contaminated area can be captured by using a pumping well (located in the cell [row, column] = [12, 6]) penetrating in the first model layer with a pumping rate of $0.0025\ m^3/s$. This low pumping rate is possible because of the low groundwater flow velocity within the zone around the contaminated area.

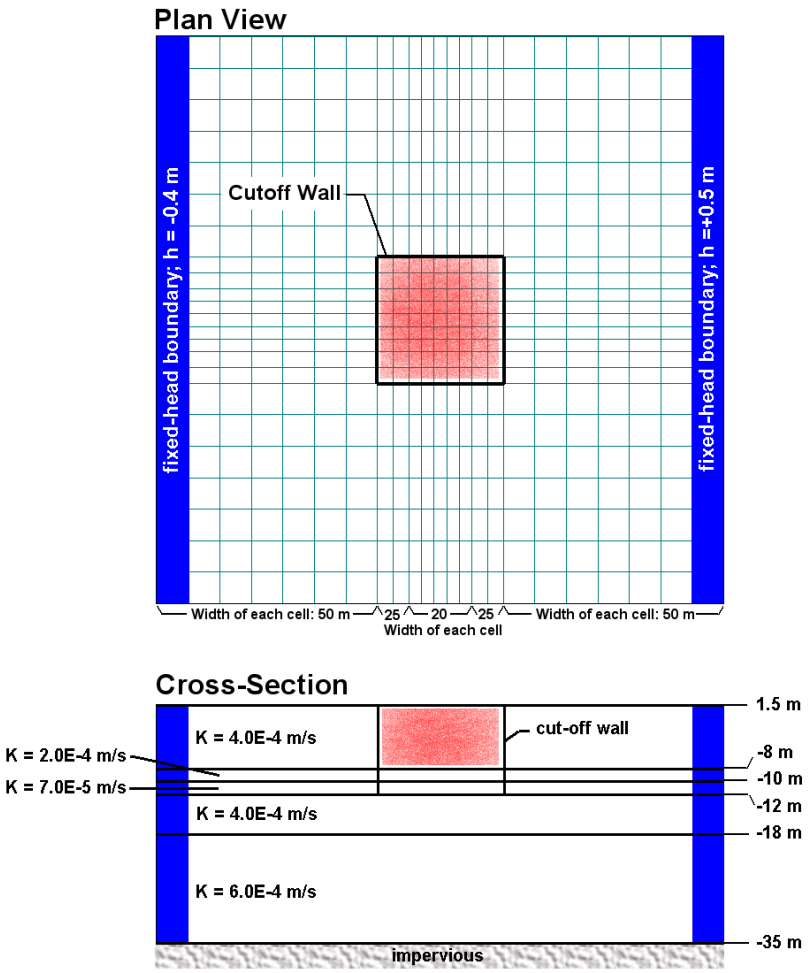


Fig. 5.42. Model grid and boundary conditions

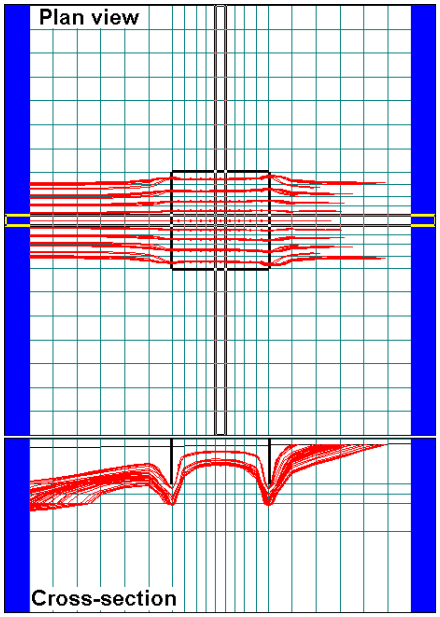


Fig. 5.43. Plan and cross-sectional views of flowlines. Particles are started from the contaminated area. The depth of the cutoff wall is -8 m.

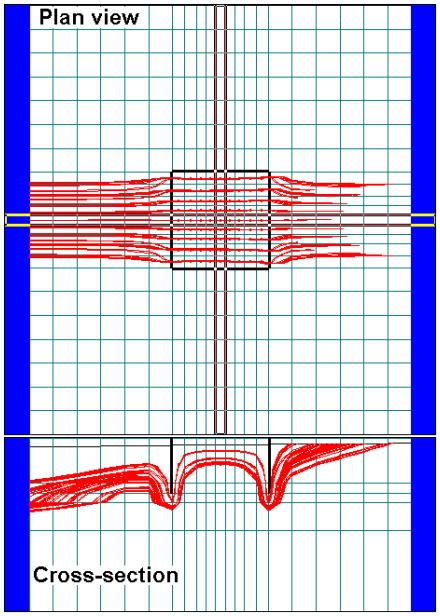


Fig. 5.44. Plan and cross-sectional views of flowlines. Particles are started from the contaminated area. The depth of the cutoff wall is -10 m

5.4.5 Compaction and Subsidence

Folder: *pmdir*\examples\geotechniques\geo5

Overview of the Problem

Fig. 5.45 shows a plan view and a cross section through an aquifer, which consists of three stratigraphic units of uniform thickness. The first unit of the aquifer is unconfined and the other units are confined. The initial hydraulic head is 43 m everywhere. The areal extent of the aquifer is assumed to be infinite large. Except a confining bed (clay) in the second unit, the sandy sediments of the aquifer are homogeneous, horizontally isotropic with an average horizontal hydraulic conductivity of 0.0001 m/s and vertical hydraulic conductivity of 0.00001 m/s. The specific yield of the first stratigraphic unit is 0.15. The specific storage of the aquifer is assumed to be 0.0001 [1/m]. The properties of the confining bed are:

Horizontal hydraulic conductivity =	$1 \times 10^{-6}\ [m/s]$
Vertical hydraulic conductivity =	$1 \times 10^{-7}\ [m/s]$
Elastic specific storage =	$0.002\ [1/m]$
Inelastic specific storage =	$0.006\ [1/m]$

To construct a new building, an excavation pit with the size ($200\ m \times 100\ m$) is required. The bottom elevation of the pit is 40 m. The pit must be held dry for one year. The task is to calculate the required withdrawal rate for keeping the pit dry and the delineate the distribution of subsidence after one year.

Modeling Approach and Simulation Results

The aquifer is simulated using a grid of 3 layers, 36 columns and 36 rows. The extent of the model grid is fairly large. Each model layer represents a stratigraphic unit. The layer type 3: confined/unconfined (Transmissivity varies) can be used for all layers, as layers of this type switch between confined and unconfined automatically. In the Layer Property dialog box, the Interbed storage flag for the second layer is checked. The pit is modeled as fixed-head boundary with the hydraulic head h = $40\ m$. The compaction (and thus the land surface subsidence) of the confining bed is modeled using the Interbed Storage package.

A transient flow simulation with one stress period and 30 time steps has been carried out. The length of the stress period is one year ($= 3.1536 \times 10^7$ seconds). The required withdrawal rate changes with time and can be calculated by using the water budget calculator (by assigning the subregion number 1 to the pit). For the first time step, the required withdrawal rate is $0.0134\ m^3/s \simeq 48.2\ m^3/h$. For the last time step, it is reduced to $0.0066 m^3/s \simeq 23.76 m^3/h$. The distribution of the subsidence caused by this withdrawal rate can be obtained by using the Results Extractor tool. Fig. 5.46 shows the contours of the land surface subsidence for the last time step. The maximum subsidence is about $0.11\ m$.

For detailed description of the Interbed Storage package and the calculation of compaction and subsidence, refer to Leake and Prudic [78], which includes two test cases. We have rebuilt the test cases and saved them in *pmdir*\examples\geotechniques\geo5a\ and *pmdir*\examples\geotechniques\geo5b\

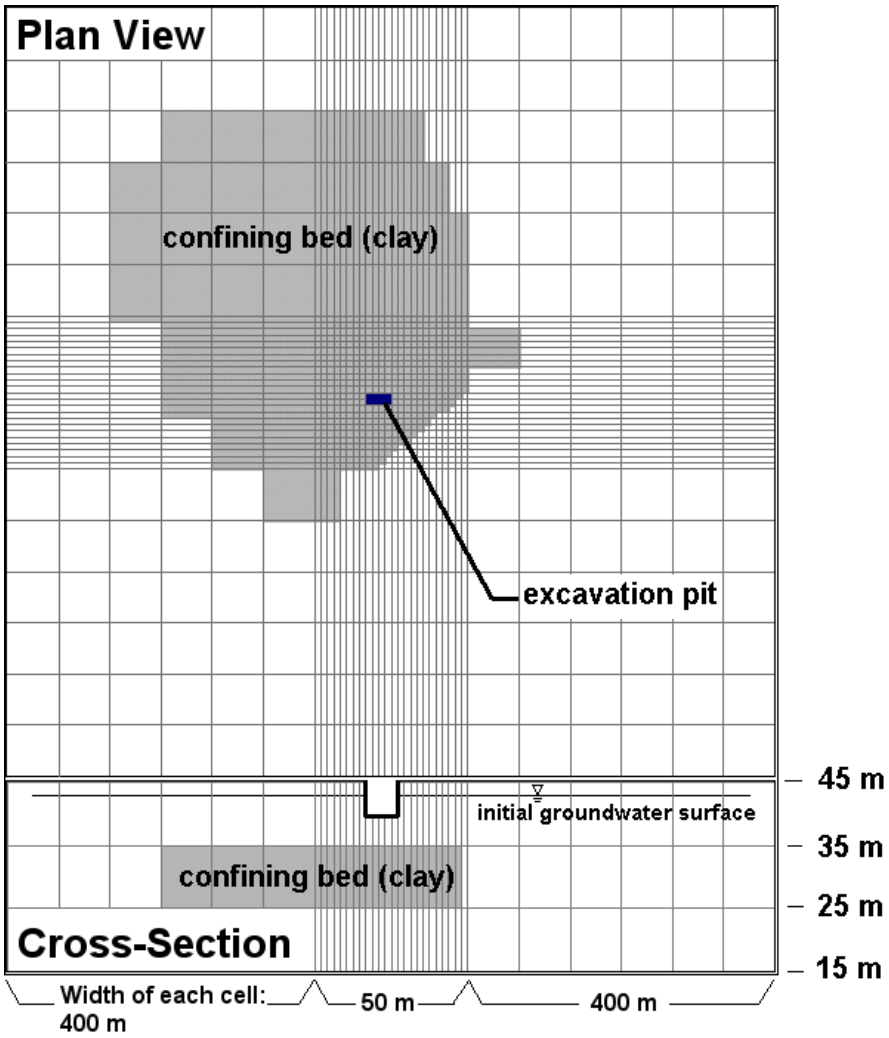


Fig. 5.45. Model grid and boundary conditions

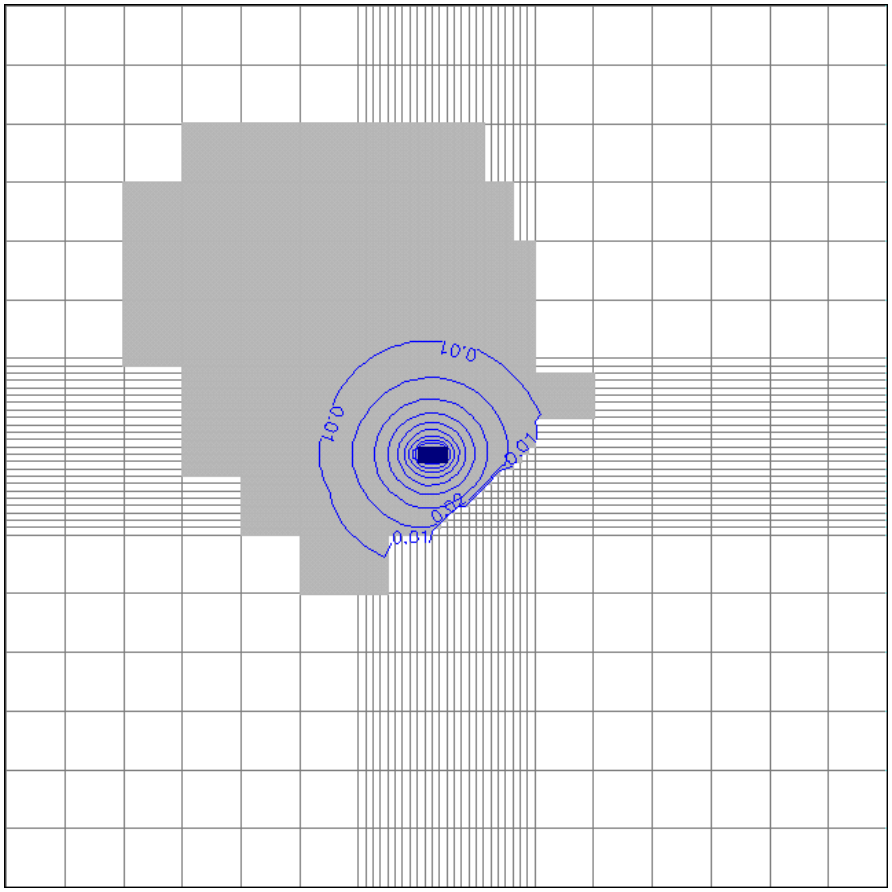


Fig. 5.46. Distribution of the land surface subsidence (maximum 0.11 m)

5.5 Solute Transport

5.5.1 One-dimensional Dispersive Transport

Folder: *pmdir*\examples\transport\transport1

Overview of the Problem

This example demonstrates the use of the numerical transport model and compares the numerical results with an analytical solution.

A uniform flow with a hydraulic gradient of 0.2% exists in a sand column. The hydraulic conductivity of the sand column is $100\ m/d$. The effective porosity is 0.2. The longitudinal dispersivity is $1\ m$. A pollutant mass of 1 gram is injected into the sand column instantaneously.

The task is to construct a one-dimensional numerical model and calculate the breakthrough curve (time series curve of concentration) at $20\ m$ downstream of the injection point. Calculate the breakthrough curve by using a longitudinal dispersivity of 4 m and compare these two curves. Will the peak arrival time of the concentration be changed if only the longitudinal dispersivity is changed?

Modeling Approach and Simulation Results

The numerical model of this example consists of one layer, one row and 51 columns. The thickness of the layer and the width of the row and column is 1 m. To obtain a hydraulic gradient of 0.2%, the first cell and the last cell of the model are specified as fixed-head cells with initial hydraulic heads of $1.1\ m$ and $1.0\ m$, respectively. The initial head of all other cells is $1.0\ m$. A steady state flow simulation is carried out for a stress period length of 100 days.

The injected mass of 1 $[g]$ is simulated by assigning an initial concentration of 5 $[g/m^3]$ to the cell [1, 1, 10]. Using the Concentration Observation dialog box, an observation borehole is set in the center of the cell [1, 1, 30]. The breakthrough curves for the dispersivity values of $1\ m$ and 4 m are shown in Fig. 5.47. It is interesting to see that the concentration peak arrives earlier (with a lower concentration value) when the value of dispersivity is higher. At the first glance, this result is somewhat confusing because the center of mass should travel with the same velocity, regardless of the value of dispersivity. Because of a higher dispersivity, the front of the concentration plume travels faster and at the same time the intensity of the concentration drops faster. This combination causes this phenomenon.

Analytical solutions for solute transport involving advection, dispersion and first-order irreversible decay in a steady-state uniform flow field are available in many text books, for example Javandel and others [68], Kinzelbach [69] or Sun [110]. A computer program for the analytical solutions of 1-D and 2-D solute transport for point-like pollutant injections is provided by Rausch [99] and included in the folder \Source\analytical solution\ of the companion CD-ROM. This program is written in BASIC. Try to use this program to compare the analytical and numerical solutions!

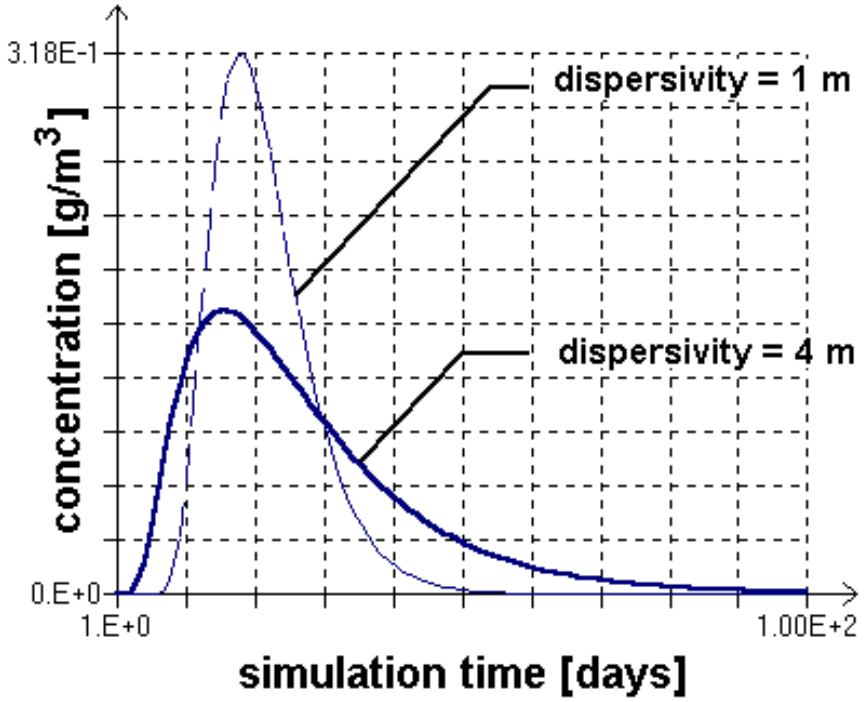


Fig. 5.47. Comparison of the calculated breakthrough curves with different dispersivity values

5.5.2 Two-dimensional Transport in a Uniform Flow Field

Folder: *pmdir*\examples\transport\transport2

Overview of the Problem

In this example, transport of solute injected continuously from a point source in a steady state uniform flow field should be simulated. The available parameters are listed below.

Layer thickness	$10\ m$
Groundwater seepage velocity	$l/3\ m/day$
Effective porosity	0.3
Longitudinal dispersivity	$10\ m$
Ratio of transverse to longitudinal dispersivity	0.3
Volumetric injection rate	$1\ m^3/day$
Concentration of the injected water	$1000\ ppm$

The task is to construct a 2D-model and use MT3DMS to calculate the concentration distribution at the end of a 365 day simulation period.

Modeling Approach and Simulation Results

A numerical model consisting of 1 layer, 31, rows, and 46 columns, and was constructed to simulate the problem. A regular grid spacing of $10\ m$ is used for each column and row. The configuration of the model is shown in Fig. 5.48. The model layer is simulated as a confined layer. The top and bottom of the model layer are at an elevation of 10 m and 0 m, respectively. To simulate the groundwater seepage velocity of $1/3\ m/day$, fixed-head boundaries (with h = $11\ m$ and h = $10\ m$) are assigned to the west and east side of the model. The horizontal hydraulic conductivity is $45\ m/day$.

The flow field was first calculated by MODFLOW. The third order TVD scheme was used in the simulation for the advection term; and the GCG solver is used to solve the system equations. The contour map of the concentration field at the end of the 365 day simulation period obtained for this example is shown in Fig. 5.49. An analytical solution for this problem is given by Wilson and Miller [116]. The analytical solution is applicable only under the assumption that (1) the aquifer is relatively thin, so that instantaneous vertical mixing can be assumed; (2) the injection rate is insignificant compared with the ambient uniform flow.

Fig. 5.50 shows the breakthrough curves at an observation well located 60 m downstream of the injection well. The analytical solution is obtained by using the computer program by Rausch [99] included in the folder \Source\analytical solution\ of the companion CD-ROM. Fig. 5.51 compares the analytical solution with the numerical solution obtained by using the upstream finite difference method. The

numerical dispersion is significant when the upstream finite difference method is used to solve the advection term.

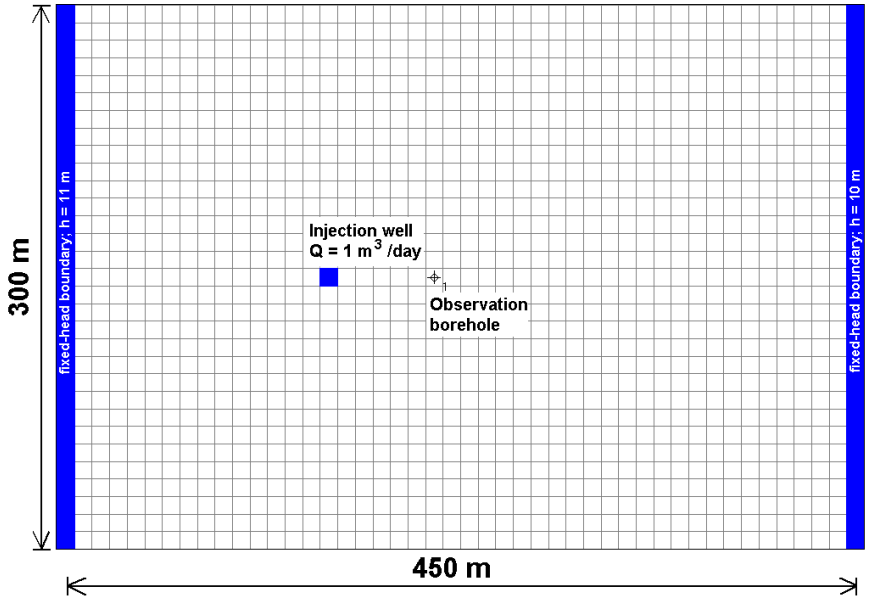


Fig. 5.48. Configuration of the model and the location of an observation borehole

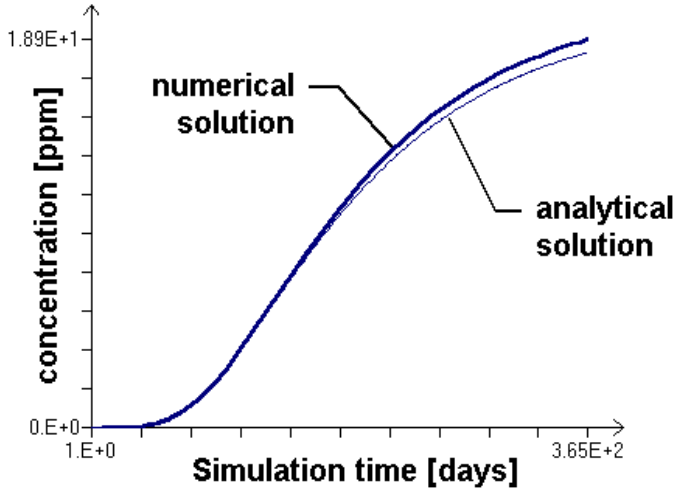


Fig. 5.50. Comparison of the breakthrough curves at the observation borehole. The numerical solution is obtained by using the 3rd order TVD scheme.

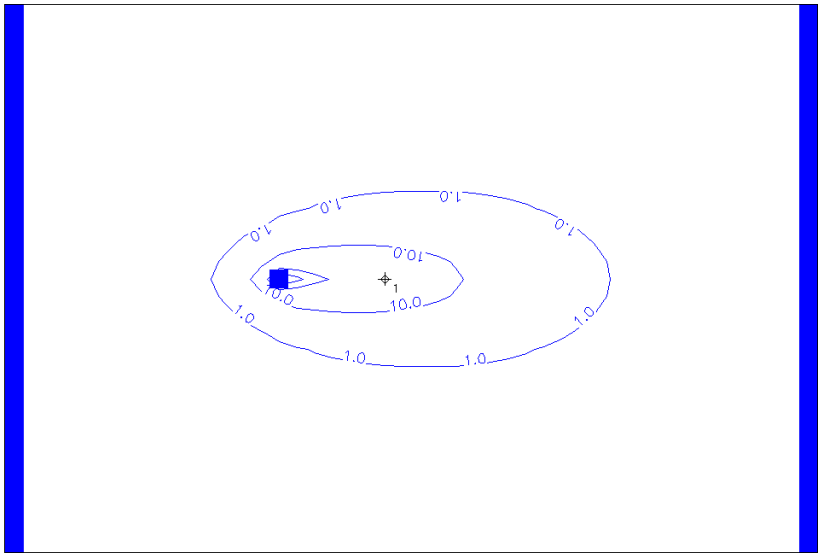


Fig. 5.49. Calculated concentration distribution

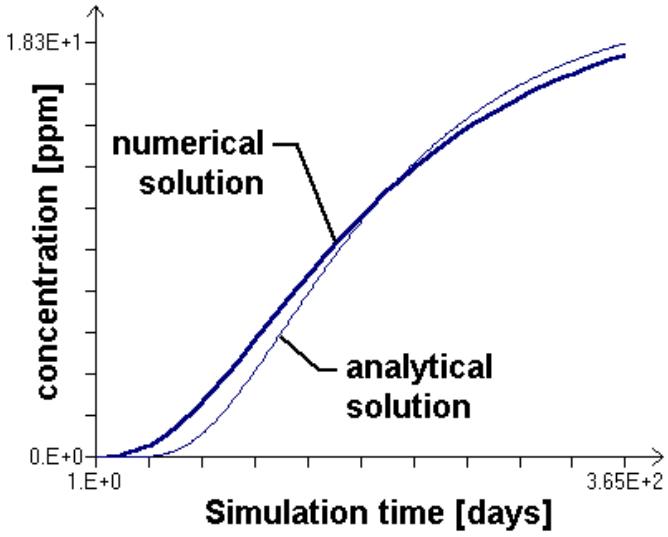


Fig. 5.51. Comparison of the breakthrough curves at the observation borehole. The numerical solution is obtained by using the upstream finite difference method.

5.5.3 Monod Kinetics

Folder: *pmdir*\examples\transport\transport3

Overview of the Problem

The example problem considered in this section is adapted from Zheng [122]. It involves one-dimensional transport from a constant source in a uniform flow field. The model parameters used in the simulation are given below.

Cell width along columns (I-direction)	$1\ m$
Cell width along rows (J-direction)	$10\ m$
Layer thickness (K-direction)	$1\ m$
Longitudinal dispersivity	$10\ m$
Groundwater seepage velocity	$0.24\ m/day$
Effective Porosity	0.25
Simulation time length	$2000\ days$

Three simulations using different parameters for the Monod kinetics as given below need to be carried out. Note that these reaction parameters are intended for demonstration purposes only and have no particular physical relevance.

Case 1:	$M_t \cdot \mu_{max} = 2\ mg/liter/day$	$K_s = 1000\ mg/liter$
Case 2:	$M_t \cdot \mu_{max} = 2 \times 10^{-3}\ mg/liter/day$	$K_s = 1\ mg/liter$
Case 3:	$M_t \cdot \mu_{max} = 2 \times 10^{-3}\ mg/liter/day$	$K_s = 0.001\ mg/liter$

Modeling Approach and Simulation Results

The model grid consists of 1 layer, 1 row, and 101 columns. In the flow model, the first and last columns are constant-head boundaries. To establish the required uniform hydraulic gradient, the initial hydraulic head values of $70\ m$ and $10\ m$ are assigned to the first and last columns, respectively. In the transport model, the first column is a constant-concentration boundary with a concentration value of $1.0\ mg/liter$. The last column is sufficiently far away from the source to approximate a semi-infinite one-dimensional flow domain.

Fig. 5.52 shows the simulation results. For Case 1, the Monod kinetics should approach a first-order reaction since K_s is three orders greater than the maximum concentration in the aquifer. Indeed, the calculated concentration profile with the Monod kinetics is nearly identical to the solution for the same transport problem but assuming a first-order reaction with the rate coefficient $\lambda = M_t \cdot \mu_{max}/K_s = 2 \times 10^{-3}\ day^{-1}$. Case 2, with K_s in the same order as the aquifer concentrations, shows the mixed-order characteristics of the Monod kinetics. In Case 3, the Monod

kinetics approaches a zero-order reaction, i.e., $\partial C/\partial t = M_t \cdot \mu_{max}$, since K_s is negligible compared to the concentrations in the aquifer.

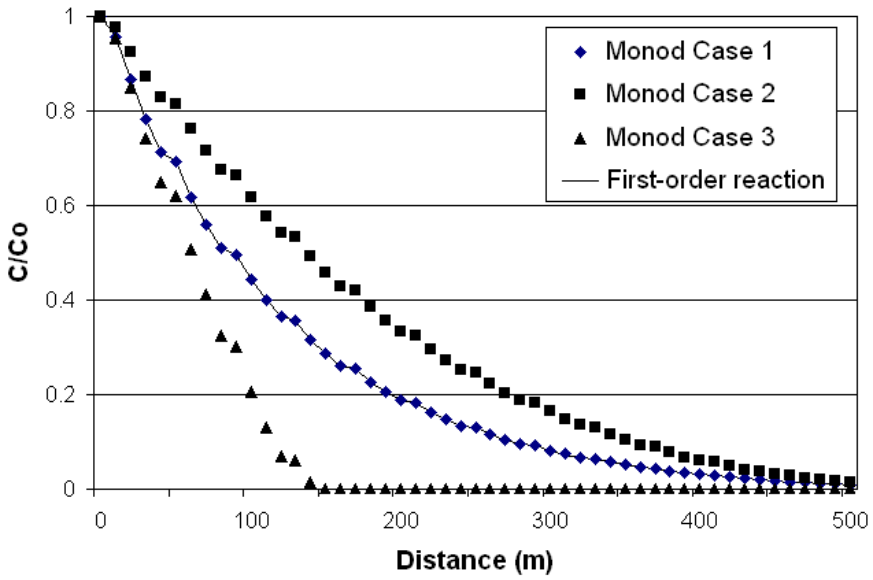


Fig. 5.52. Calculated concentration values for one-dimensional transport from a constant source in a uniform flow field.

5.5.4 Instantaneous Aerobic Biodegradation

Folder: *pmdir*\examples\transport\transport4

Overview of the Problem

The example problem considered in this section is adapted from Zheng [122] and is similar to the model described in Section 5.5.2. The problem involves two-dimensional transport from a continuous point source in a uniform flow field. The point source has a volumetric injection rate of $1\ m^3/day$ and the injected water contains hydrocarbon (species 1) with a constant concentration of 1000 ppm. The background concentration of oxygen (species 2) in the aquifer is $9\ ppm$. Hydrocarbon and oxygen are assumed to react instantaneously; the stoichiometric ratio for the reaction is approximately 3.0, i.e., one mass unit of hydrocarbon reacts with three mass unit of oxygen. The other model parameters used in the simulation are given below.

Cell width along columns (I-direction)	$10\ m$
Cell width along rows (J-direction)	$10\ m$
Layer thickness (K-direction)	$10\ m$
Groundwater seepage velocity	$0.3333\ m/day$
Effective Porosity	0.3
Longitudinal dispersivity	$10\ m$
Ratio of transverse to longitudinal dispersivity	0.3
Volumetric injection rate	$1\ m^3/day$
Simulation time	$730\ days$

The concentration distributions of hydrocarbon and oxygen after a simulation period of 730 days (2 years) need to be calculated.

Modeling Approach and Simulation Results

The model grid is aligned with the flow direction along the x-axis and consists of 1 layer, 31 rows, and 46 columns. The flow model is surrounded by constant-head boundaries on the east and west borders and no-flow boundaries on the north and south borders. To establish the required uniform hydraulic gradient, the head values $11\ m$ and $10\ m$ are assigned to the first and last columns, respectively.

The point source is simulated using an injection well located at column 11 and row 16. The injection rate is sufficiently small so that the flow field remains approximately uniform. The background oxygen concentration is modeled by setting the initial concentration of species 2 to $9\ ppm$ in all model cells and by assigning $9\ ppm$ to the species 2 concentration of the inflow from the constant-head boundary.

The concentrations for hydrocarbon and oxygen at the end of the two-year simulation period are calculated by RT3D and shown in Figures 5.53 and 5.54. The maximum concentration of hydrocarbon is approximately $50\ ppm$ at the injection point

(Fig. 5.53). The oxygen plume is depleted where the concentration of hydrocarbon is above zero (Fig. 5.54). For this example, the TVD scheme is chosen for solving the advection term while all other terms are solved by the explicit finite-difference option. The mass balance discrepancies for both species are less than $10^{-4}\%$. The calculated hydrocarbon and oxygen plumes are nearly identical to those calculated using MT3D99 [122].

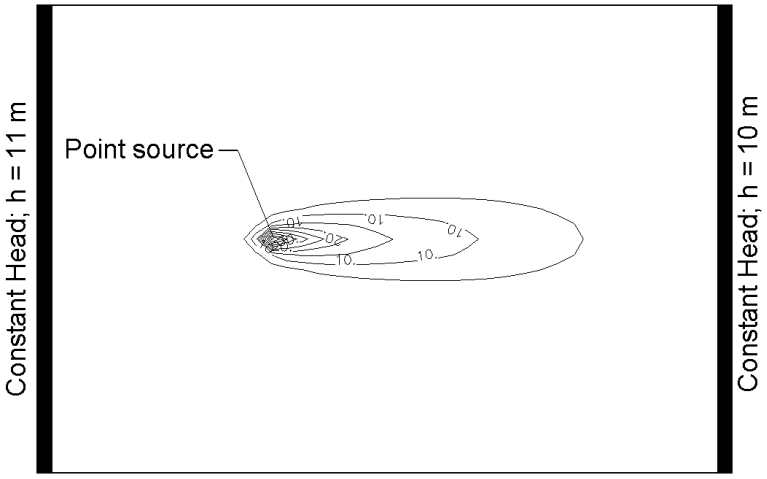


Fig. 5.53. Calculated concentration values of hydrocarbon

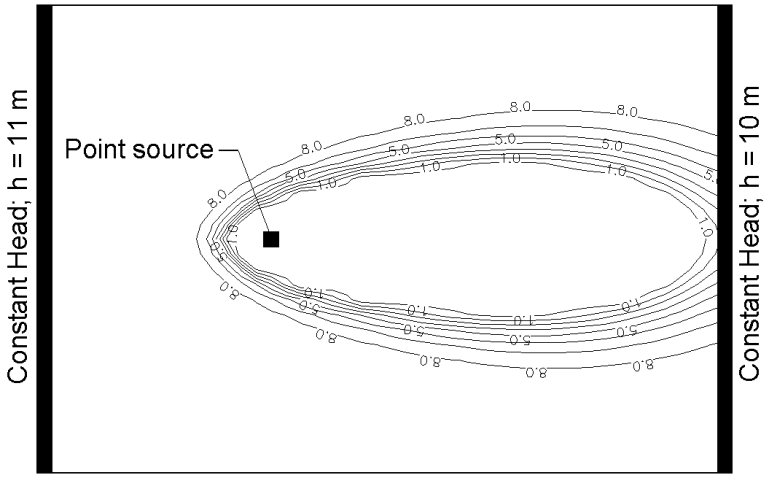


Fig. 5.54. Calculated concentration values of oxygen

5.5.5 First-Order Parent-Daughter Chain Reactions

Folder: *pmdir*\examples\transport\transport5

Overview of the Problem

The example problem is adapted from Zheng [122]. It involves one-dimensional transport of three species in a uniform flow field undergoing first-order sequential transformation. The model parameters used in this example are identical to those used in Clement [25] for the PCE–TCE–DCE–VC sequential transformation and are given below.

Cell width along columns (I-direction)	$1\ cm$
Cell width along rows (J-direction)	$0.5\ cm$
Layer thickness (K-direction)	$1\ cm$
Longitudinal dispersivity	$1.8\ cm$
Groundwater seepage velocity	$0.1\ cm/hr$
First-order reaction rate for PCE (species 1)	$0.05\ hr^{-1}$
First-order reaction rate for TCE (species 2)	$0.03\ hr^{-1}$
First-order reaction rate for DCE (species 3)	$0.02\ hr^{-1}$
First-order reaction rate for VC (species 4)	$0.01\ hr^{-1}$
Retardation factor for PCE (species 1)	2
Yield coefficient between PCE and TCE (Y1/2)	0.792
Yield coefficient between TCE and DCE (Y2/3)	0.738
Yield coefficient between DCE and VC (Y3/4)	0.644
Simulation time	$200\ hours$

Modeling Approach and Simulation Results

The model grid consists of 1 layer, 1 row, and 101 columns. In the flow model, the first and last columns are constant-head boundaries. To establish the required uniform hydraulic gradient, the head values $0.5\ cm$ and $0\ cm$ are assigned to the first and last columns, respectively.

In the transport model, the first column is a constant-concentration boundary for all species with the concentration values equal to $1.0\ mg/liter$ for PCE (species 1) and zero for other species. The last column is sufficiently far away from the source to approximate a semi-infinite one-dimensional flow domain. The initial concentration values for all species are assumed to be zero. The retardation factor of 2 is simulated by assigning n_e = 0.1, bulk density $\rho_b = 1000kg/m^3$ and distribution coefficient $K_d = 0.0001m^3/kg$, as the retardation factor R is calculated by

$$R = 1 + \frac{\rho_b}{n_e} \cdot K_d \tag{5.3}$$

Fig. 5.55 shows the concentration distributions calculated by RT3D for all four species at the end of the 200-hour simulation period. The calculated values agree

closely with the solutions of MT3D99 [122], which are not shown in the figure since the curves are nearly identical. It can be seen that as PCE (species 1) is transported from the source, its mass lost to decay becomes the source for TCE (species 2), some of which is, in turn, transformed into DCE (species 3), and then VC (species 4).

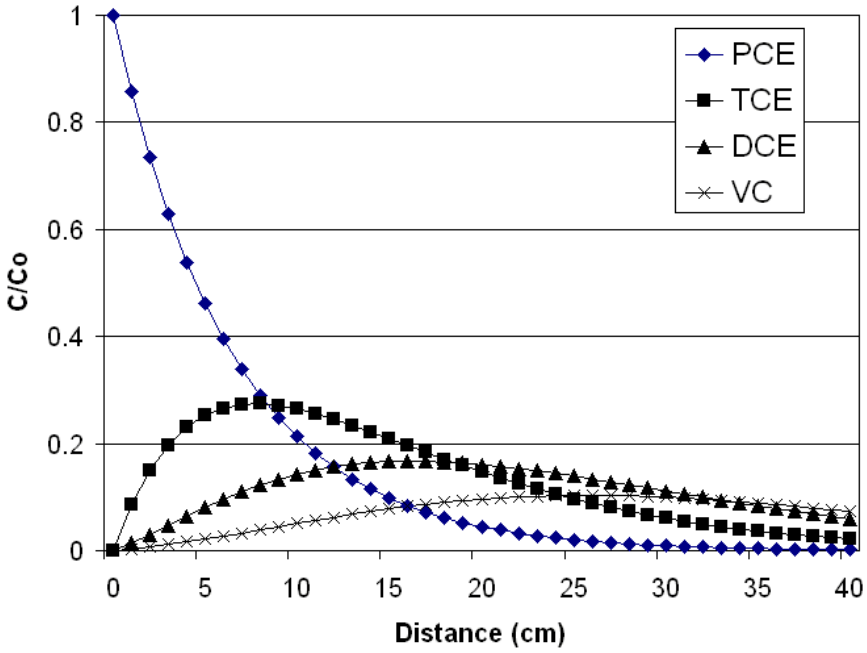


Fig. 5.55. Comparison of calculated concentration values of four species in a uniform flow field undergoing first-order sequential transformation

5.5.6 Benchmark Problems and Application Examples from Literature

Folder: *pmdir*\examples\transport\

Overview of the Problem

To test the accuracy and performance of the MT3D/MT3DMS and MOC3D codes, several benchmark problems and application examples are introduced in the user's guides of MT3D [117], MT3DMS [121], and MOC3D [74]. You can find these documents on the folders \document\mt3d\, \document\mt3dms\, and \document\moc3d\ of the companion CD-ROM.

Modeling Approach and Simulation Results

We have rebuilt most of the benchmark problems of MT3D/MT3DMS and MOC3D by using **PM**. These models are saved in the sub-folders under \path\examples\transport\ listed below. All these models are ready-to-run. It is recommended that the users try these test problems first to become familiarized with the various options before applying MT3D/MT3DMS or MOC3D to solve their own problems.

Folder	Description
\transport6\	This model is described in Section 7.5 of the manual of MT3DMS. A numerical model consisting of 1 layer, 31 rows, and 31 columns is used to simulate the two-dimensional transport in a radial flow field; numerical results were compared with the analytical solution of Moench and Ogata [88].
\transport7\	This model is described in Section 7.6 of the manual of MT3DMS. A numerical model consisting of 1 layer, 31 rows, and 31 columns is used to simulate the concentration change at the injection/abstraction well; numerical results were compared with the approximate analytical solution of Gelhar and Collins [48].
\transport8\	This model is described in Section 7.7 of the manual of MT3DMS. A numerical model consisting of 8 layers, 15 rows, and 21 columns is used to solve three-dimensional transport in a uniform flow field. The point source was simulated at layer 7, row 8, and column 3. Numerical results were compared with the analytical solution of Hunt [67].
\transport9\	This model is described in Section 7.9 of the manual of MT3DMS. This example illustrates the application of MODFLOW and MT3D/MT3DMS to a problem involving transport of contaminants in a two-dimensional heterogeneous aquifer.

Folder	Description
\transport10\	This model is described in Section 7.10 of the manual of MT3DMS. This example illustrates the application of MT3D/MT3DMS to an actual field problem involving the evaluation of the effectiveness of proposed groundwater remediation schemes.
\transport11\	This model is described in the section MODEL TESTING AND EVALUATION – One-Dimensional Steady Flow of the user's guide of MOC3D. A numerical model consisting of 1 layer, 1 row, and 122 columns is used to simulate one-dimensional transport having a third-type source boundary condition in a steady-state flow field; numerical results were compared with the analytical solution of Wexler [114].
\transport12\	This model is described in the section MODEL TESTING AND EVALUATION – Three-Dimensional Steady Flow of the user's guide of MOC3D. A numerical model consisting of 40 layers, 32 rows, and 12 columns is used to simulate three-dimensional transport having a permanent point source in a steady-state flow field; numerical results were compared with the analytical solution of Wexler [114].
\transport13\	This model is described in the section MODEL TESTING AND EVALUATION – Two-Dimensional Radial Flow and Dispersion of the user's guide of MOC3D. A numerical model consisting of 1 layer, 30 rows, and 30 columns is used to simulate two-dimensional transport having a permanent point source in a steady-state radial flow field; numerical results were compared with the analytical solution given by Hsieh [65].
\transport14\	This model is described in the section MODEL TESTING AND EVALUATION – Point Initial Condition in Uniform Flow of the user's guide of MOC3D. A numerical model consisting of 26 layers, 26 rows, and 26 columns is used to simulate three-dimensional transport having an initial point source in a parallel steady-state flow at 45 degrees to the x-direction; numerical results were com-pared with the analytical solution given by [114]. The point source was simulated at layer 12, row 4, column 4.

5.6 PHT3D Examples

Folder: *pmdir*\examples\PHT3D\

Overview of the Problem

Twelve documented examples, complete with problem statements, input data sets, and discussion of results are presented in the user's guide of PHT3D [97]. Those examples are designed to use as benchmark problems as well as to demonstrate the application of PHT3D. A complete list of the examples is given in Table 5.7.

Modeling Approach and Simulation Results

Most of the models described in the user's guide of PHT3D were created or re-created by using the present version of **PM**. You can find the models in sub-folders under path\examples\PHT3D\.

Table 5.7 PHT3D Examples

Example	Description
EX01	Single Species Transport with Monod Kinetics
EX02	Transport and mineral precipitation/dissolution
EX03	Migration of precipitation/dissolution fronts
EX04	Cation exchange - flushing of a sodium-potassium nitrate solution with calcium chloride
EX05	Cation exchange during artificial recharge
EX06	Cation exchange and precipitation/dissolution during tenside injection
EX07	Kinetic, sequential/parallel degradation of multiple species
EX08	Kinetic, sequential degradation of chlorinated hydrocarbons
EX09	Kinetic degradation of BTEX using multiple electron acceptors
EX10	Dissolution, degradation and geochemical response
EX11	Transport and surface complexation of uranium
EX12	Modelling of an oxidation experiment with pyrite/calcite/exchangers/organic matter containing sand

5.7 SEAWAT Examples

Folder: *pmdir*\examples\SEAWAT\

Overview of the Problem

The examples presented here are based on the example problem described in the user's guide of SEAWAT_V4 [77]. The example problem consists of a two-dimensional cross section of a confined coastal aquifer initially saturated with relatively cold seawater at a temperature of $5\,^{\circ}\mathrm{C}$. Warmer freshwater with a temperature of $25\,^{\circ}\mathrm{C}$ is injected into the coastal aquifer along the left boundary to represent flow from inland areas. The warmer freshwater flows to the right, where it discharges into a vertical ocean boundary. The ocean boundary is represented with hydrostatic conditions based on a fluid density calculated from seawater salinities at $5\,^{\circ}\mathrm{C}$. No-flow conditions are assigned to the top and bottom boundaries. A complete list of the input values used for the problem is given in table 5 of the SEAWAT_V4 user's guide. This problem is a simplified representation of what might occur in a coastal carbonate platform.

Modeling Approach and Simulation Results

Five cases of the example problem described in the user's guide of SEAWAT_V4 were re-created by using the present version of **PM** and are given in Table 5.8. You can find the models in sub-folders under path\examples\SEAWAT\.

Table 5.8 SEAWAT Examples

Example	Description
CASE1	Variable-density simulation in which the fluid density is a function only of salinity.
CASE2	Variable-density simulation in which the fluid density is a function of salinity and temperature.
CASE3	Variable-density simulation in which the fluid density is a function of salinity and temperature while considering heat conduction in the simulation.
CASE4	Variable-density simulation in which the fluid density is a function of salinity and temperature while considering heat conduction and thermal equlibration between the fluid and the solid matrix.
CASE5	Variable-density simulation in which the fluid density is a function of salinity and temperature while considering heat conduction and thermal equlibration between the fluid and the solid matrix as well as heat conduction at the seawater boundary.

5.8 Miscellaneous Topics

5.8.1 Using the Field Interpolator

Folder: *pmdir*\examples\misc\misc1

Overview of the Problem

This example illustrates the use of the Field Interpolator. Fig. 5.56 shows the plan view of the model area, the model grid and the locations of measurement points. The model grid consists of 1 layer, 70 rows, and 60 columns. The measured hydraulic heads and the coordinates of the measurement points are saved in *pmdir*\examples\misc\misc1\measure.dat. To obtain the starting head distribution of a flow simulation, the measured hydraulic heads should be interpolated to each model cell.

Modeling Approach and Simulation Results

The starting heads are interpolated to model cells using the four interpolation methods provided by the Field Interpolator. The interpolation results are shown in the form of contours in Figures 5.57 – 5.60. The octant search method with *Data Per Sector* = 1 is used by all gridding methods. A weighting exponent of $F = 2$ is used by Shepard's inverse distance method. The Kriging method uses the linear variogram model with $c_0 = 0$ and $\alpha = 1$. There is no significant difference observed in these fig-

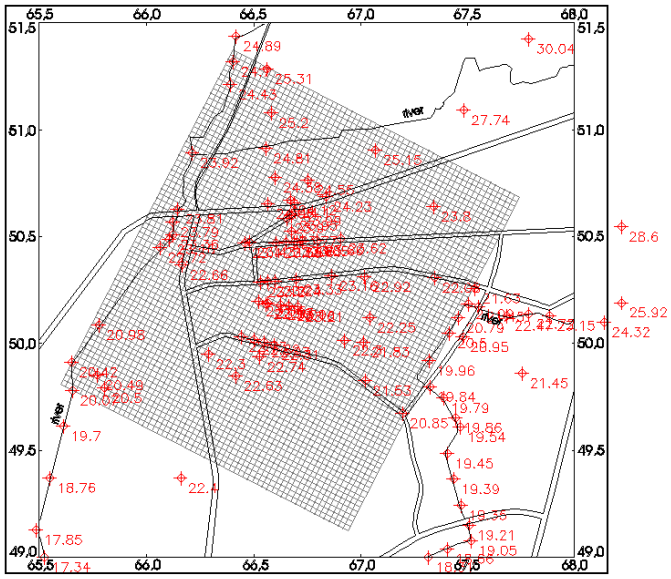


Fig. 5.56. Model domain and the measured hydraulic head values

ures when sufficient data points are available. The major difference is observed in the southern part of the model area, where only one measurement point is found and the system is not well conditioned.

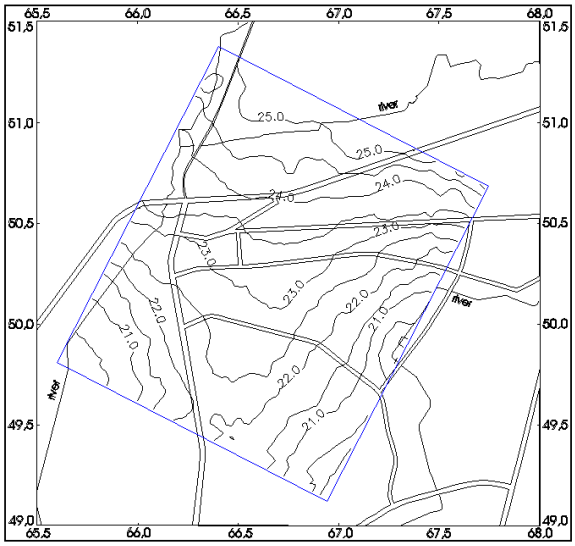


Fig. 5.57. Contours produced by Shepard's inverse distance method

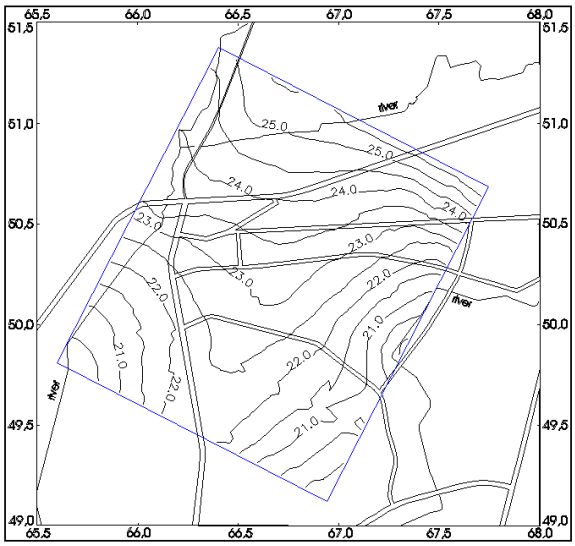


Fig. 5.58. Contours produced by the Kriging method

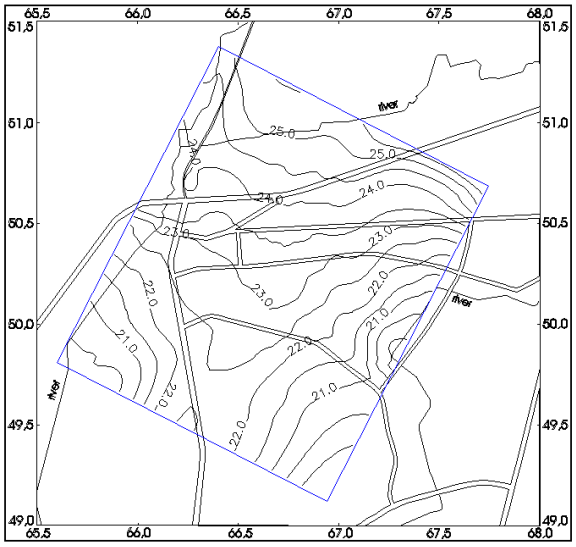


Fig. 5.59. Contours produced by Akima's bivariate interpolation

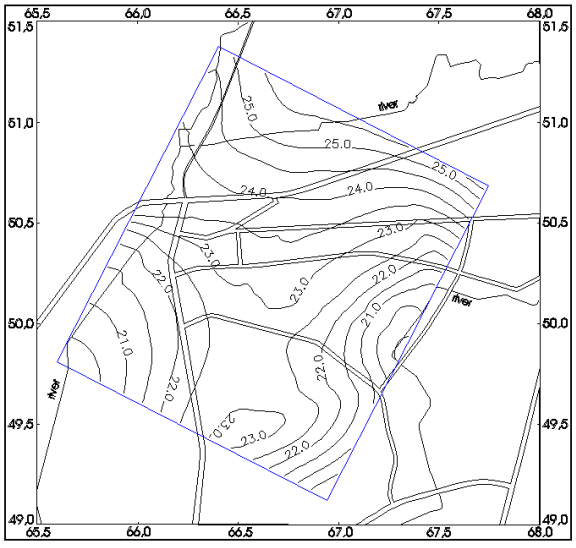


Fig. 5.60. Contours produced by Renka's triangulation algorithm

5.8.2 An Example of Stochastic Modeling

Folder: *pmdir*\examples\misc\misc2\

Overview of the Problem

Aquifer remedial measures are often designed by means of groundwater models. Model results are usually uncertain due to the imperfect knowledge of aquifer parameters. We are uncertain about whether the calibrated values of parameters represent the real aquifer system. We never know the actual small-scale distribution of some parameters, e.g. hydraulic conductivity or recharge. Thus, all groundwater models involve uncertainty. Stochastic models are often employed to take into account uncertainty. In the stochastic modeling approach, the model parameters appear in the form of probability distributions of values, rather than as deterministic sets.

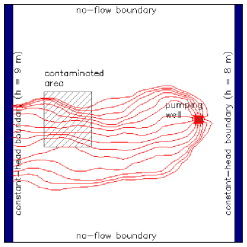
We use the aquifer described in Section 4.1 to illustrate the concept of stochastic modeling. Using a two-dimensional approach to model the aquifer, we may use the Field Generator to create log-normal correlated distributions of the horizontal hydraulic conductivity. The mean horizontal hydraulic conductivity of the aquifer is equal to $(4 \times 0.0001 + 6 \times 0.0005)/10 = 3.4 \times 10^{-4}\ m/s$. The standard deviation is assumed to be $\sigma = 0.5$. A correlation length of $60\ m$ is used.

In Section 4.1, the pumping rate of the well was determined such that the contaminated area lies within the capture zone of the well. When different realizations of the heterogeneous distribution of hydraulic conductivity are introduced, it is obvious that the capture zone not always covers the entire contaminated area. The safety criterion for the measure can be defined as the percentage of the covered area in relation to the entire contaminated area. The expected value of the safety criterion can be obtained from stochastic simulation.

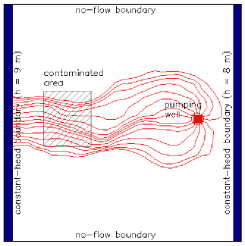
Modeling Approach and Simulation Results

Using the Field Generator, log-normal distributions of the horizontal hydraulic conductivity are generated and stored in ASCII Matrix files. First, each generated realization is imported into the horizontal hydraulic conductivity matrix, then a flow simulation is performed. The capture zone of the pumping well, as well as pathlines, are computed with PMPATH. The resulting safety criterion is obtained by a Monte Carlo simulation. This implies that many realizations of the parameter field are produced and used in the flow simulation.

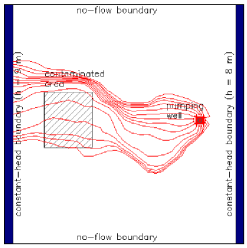
Fig. 5.61 shows results of five realizations and the calculated mean safety criterion. The mean safety criterion is the sum of safety criteria divided by the number of realizations. A large number of realizations may be required for the mean safety criterion to converge.



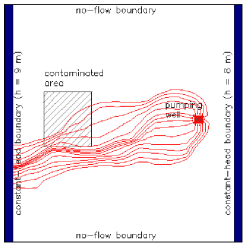
Realization 1
Safety Criterion = 85 %
Mean Safety Criterion = 85%



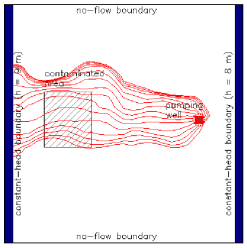
Realization 2
Safety Criterion = 87 %
Mean Safety Criterion = 86%



Realization 3
Safety Criterion = 97 %
Mean Safety Criterion = 89.7%



Realization 4
Safety Criterion = 48 %
Mean Safety Criterion = 79.3%



Realization 5
Safety Criterion = 93 %
Mean Safety Criterion = 82%

Fig. 5.61. Calculation of the mean safety criterion by the Monte Carlo method

6

Supplementary Information

6.1 Limitation of PM

This section gives the size limitation of **PM**. Refer to the documentation of individual packages for their assumptions, applicability and limitations.

6.1.1 Data Editor

Maximum number of layers = 300
Maximum number of stress periods = 1000
Maximum number of cells along rows or columns = 2000
Maximum number of cells in a layer = 1000000
Maximum number of polygons in a layer = 20
Maximum number of vertex nodes of a polygon = 40
Maximum number of stream segments = 1000
Maximum number of tributary segments of each stream segment = 10
Maximum number of reservoirs = 20
Maximum number of observed stages of each reservoir = 200
Maximum number of estimated parameters = 500
Maximum number of species = 60

There is no limit to the polylines and number of wells, general-head boundary cells, rivers, drains, and horizontal-flow-barrier cells.

6.1.2 Boreholes and Observations

No limit to the maximum number of boreholes
Maximum number of observations for each borehole = 4000

6.1.3 Digitizer

Maximum number of digitized points = 50000

6.1.4 Field Interpolator

Maximum number of cells in a layer = 1,000,000
Maximum number of cells along rows or columns = 5000
Maximum number of input data points = 5000

6.1.5 Field Generator

Maximum number of cells in a layer = 250000
Maximum number of cells along rows or columns = 500

6.1.6 Water Budget Calculator

Maximum number of subregions = 50

6.2 File Formats

6.2.1 ASCII Matrix File

An ASCII Matrix file can be saved or loaded by the Browse Matrix dialog box (see Section 2.8.1) of the Data Editor. The Results Extractor, Field Interpolator and Field Generator save their generated data in this format.

```
File Format
1. Data: NCOL NROW
2. Data: MATRIX (NCOL, NROW)
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

- **NCOL** is the number of model columns.
- **NROW** is the number of model rows.
- **MATRIX** is a two-dimensional data matrix saved row by row. Matrix can be saved in free format. If the wrap from is used to save the matrix, each line of the matrix contains up to 20 values.

Example

If NCOL=6 and NROW=5, an ASCII Matrix file would be

```
6 5
121 152 133 144 315 516
221 252 233 244 215 216
```

```
321 352 333 344 315 316
421 452 433 444 415 416
521 552 533 544 515 516

Or

6 5
121 152 133 144 315 516 221 252 233 244 215 216
321 352 333 344 315 316 421 452 433 444 415 416
521 552 533 544 515 516
```

6.2.2 Contour Table File

A contour table file can be saved or loaded by the Environment Options dialog box (see Section 2.9.2).

```
File Format
1. Data: LABEL
2. Data: NL XXX XXX XXX XXX
```

(The following data repeats NB times)

```
3. Data: LEVEL COLOR FILL LVISIBLE LSIZE LDIS XXX XXX XXX
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

- **LABEL** is the file label. It must be PMWIN5000_CONTOUR_FILE. The file format has been changed since PMWIN 5.0.
- **NL** is the number of contour levels
- **XXX** reserved.
- **LEVEL** is the Contour level
- **COLOR** is the color used to draw the contour line; The color is defined by a long integer using the equation: color = red + green $\times$ 256 + blue $\times$ 65536, where red, green and blue are the color components ranging from 0 to 255.
- **FILL** is the color used to fill the space between the current contour and the next contour level.
- **LVISIBLE** controls the visibility of the corresponding contour. The contour is visible if LVISIBLE is TRUE.
- **LSIZE** is the appearance height of the label text in the same unit as the model.
- **LDIS** is the distance between two contour labels, in the same unit as the model.

6.2.3 Grid Specification File

The grid specification file provides the grid geometry and location details.

```
File Format
1. Data: NROW NCOL
2. Data: X Y ANGLE
3. Data: DELR(NCOL)
4. Data: DELC(NROW)
5. Data: X1 Y1
6. Data: X2 Y2
7. Data: NLAY
```

(The following data contains the top elevations of each layer. This data record repeats NLAY times if the layer top elevation has been specified)

```
8. Data: TOP
```

(The following data contains the bottom elevations of each layer. This data record repeats NLAY times if the layer bottom elevation has been specified)

```
9. Data: BOTTOM
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

- **NROW** is the number of model rows.
- **NCOL** is the number of model columns.
- **X** is the x-coordinate of the top-left corner of the model grid.
- **Y** is the y-coordinate of the top-left corner of the model grid.
- **ANGLE** is the rotation angle expressed in degrees and measured counterclockwise from the positive x-axis.
- **DELR** is the cell width along rows. Read one value for each of the NCOL columns. This is a single array with one value for each column.
- **DELC** is the cell width along columns. Read one value for each of the NROW rows. This is a single array with one value for each row.
- **X1, Y1** are the coordinates of the lower left corner of the model worksheet (see Coordinate System for details).
- **X2, Y2** are the coordinates of the upper right corner of the model worksheet (see Coordinate System for details).
- **NLAY** is the number of model layers.
- **TOP** is a 2D matrix contains the top elevation of each model cell of a model layer.
- **BOTTOM** is a 2D matrix contains the bottom elevation of each model cell of a model layer.

6.2.4 Line Map File

A line map file contains a series of polylines, each polyline is defined by the number of vertices and a series of coordinate pairs.

```
File Format
Repeat Data 1 and 2 for each polyline

1. Data: NVERTEX
```

(The following data repeats NVERTEX times)

```
2. Data: X Y
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

- **NVERTEX** is the number of vertices of a polyline
- **X** is the x-coordinate of the i-th vertex
- **Y** is the y-coordinate of the i-th vertex

6.2.5 ASCII Time Parameter File

An ASCII time parameter file can be saved or loaded by the Time Parameters dialog box (see Section 2.5.1).

```
File Format
1. Data: LABEL
2. Data: NPER ITMUNI
3. Data: Reserved Reserved Reserved Reserved
4. Data: Reserved Reserved Reserved Reserved
5. Data: Reserved Reserved Reserved Reserved
```

(The following data repeat NPER times)

```
6. Data: ACTIVE PERLEN NSTP TSMULT DT0 MXSTRN TTSMULT TRANS
7. Data: Reserved Reserved Reserved Reserved Reserved Reserved
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

- **LABEL** is the file label. It must be PMWIN_TIME_FILE
- **NPER** is the number of stress periods in the simulation

– **ITMUNI** indicates the time unit of model data. The time unit must be consistent for all data values that involve time. For example, if years is the chosen time unit, stress period length, time step length, transmissivity, etc., must all be expressed using years for their time units. Likewise, the length unit must also be consistent.

```
0 - undefined   3 - hours
1 - seconds     4 - days
2 - minutes     5 - years
```

– **ACTIVE** A stress period is active, if ACTIVE = -1. Set ACTIVE=0, if a stress period is inactive.
– **PERLEN** is the length of a stress period. It is specified for each stress period.
– **NSTP** is the number of time steps in a stress period.
– **TSMULT** is the multiplier for the length of successive time steps. The length of the first time step DELT(1) is related to PERLEN, NSTP and TSMULT by the relation DELT(1) = PERLEN(1 TSMULT)/(1 TSMULT**NSTP).
– **DT0** is the length of transport steps. If DT0=0, the length of transport steps will be determined by an automatic stepsize control procedure in MT3D.
– **MXSTRN** is the maximum number of transport steps.
– **TTSMULT** is the multiplier for the length of successive transport steps within a flow time step, if the Generalized Conjugate Gradient (GCG) solver is used and the solution option for the advection term is the upstream finite difference method.
– **TRANS** is used by MODFLOW-2000 only. A stress period is simulated in transient state is TRANS = -1, otherwise a steady-state solution will be calculated for the stress period.
– **Reserved**: Reserved for future use. Enter 0 in the file.

6.2.6 Head/Drawdown/Concentration Observation Files

The Head (or Drawdown, or Concentration) Observation dialog box uses the following four formats for saving and loading data. The formats are described in the following sections.

- **Observation Boreholes (∗.obs_borehole)** contains names and coordinates of observation boreholes.
- **Layer Proportions (∗.layer_prop)** contains the proportion values of each layer. Using the Head Observation dialog box, a Layer Proportions file can be loaded to an observation borehole at a time.
- **Observations (∗.observation)** contains observation times, observed values and weights. Using the Head Observation dialog box, an Observations file can be loaded to an observation borehole at a time.
- **Complete Information (∗.complete_obs)** contains all information mentioned above for all boreholes.

6.2.6.1 Observation Boreholes File

```
1. Data: NBOREHOLES
```

(The following data repeat for each borehole (i.e. NBOREHOLES times))

```
2. Data: OBSNAM Active x y
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

- **NBOREHOLES** is the number of observation boreholes
- **Active**: A borehole is active if Active = 1; A borehole is inactive if Active = 0.
- **x**: x coordinate of the borehole.
- **y**: y coordinate of the borehole.

6.2.6.2 Layer Proportions File

```
1. Data: NLAYERS
2. Data: PR(1) PR(2) ... PR(NLAYERS)
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

- **NLAYERS**: Number of layers in the model.
- **PR(i)**: layer proportion values for layer i.

6.2.6.3 Observations File

```
1. Data: NHOBS
```

(The following data repeat for each observation (i.e. NHOBS times))

```
2. Data: Time, HOBS, STWT
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

- **NHOBS**: number of observations
- **Time**: Observation time.
- **HOBS**: observed value at Time.
- **STWT**: For MODFLOW-2000, STWT is the statistic value for the observation. For PEST, STWT is the weighting factor for the observation.

6.2.6.4 Complete Information File

```
1. Data: PMWIN_OBSERVATION_FILE
2. Data: NBOREHOLES EVH
3. Data: Reserved Reserved Reserved Reserved
4. Data: ITT STAT_FLAG
5. Data: Reserved Reserved Reserved Reserved
```

(The following data repeat for each borehole (i.e. NBOREHOLES times))

```
6. Data: OBSNAM Active x y NHOBS
7. Data: PR(1) PR(2) ... PR(NLAYERS)
```

(The following data repeat NHOBS times for each borehole)

```
8. Data: Time, HOBS, statistic, weight
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

- The text string PMWIN_OBSERVATION_FILE must be entered literally.
- **NBOREHOLES** is the number of observation boreholes.
- **EVH**: default =1 for MODFLOW-2000, not used by PEST.
- **ITT**: default =1 for MODFLOW-2000, not used by PEST.
- **STAT_FLAG**: default =0 for MODFLOW-2000, not used by PEST.
- **OBSNAM**: name of the observation borehole, max 8 characters, blank and special characters are not allowed
- **Active**: A borehole is active if Active = 1; A borehole is inactive if Active = 0.
- **x**: x coordinate of the borehole.
- **y**: y coordinate of the borehole.
- **NHOBS**: number of observations of a borehole.
- **PR(i)**: layer proportion values for layer i.
- **NLAYERS**: Number of layers in the model.
- **Time**: Observation time.
- **HOBS**: observed value at Time.
- **Statistic**: statistic value for the observation (used by MODFLOW-2000).
- **weight**: weighting factor for the observation (used by PEST).
- **Reserved**: Reserved for future use. Enter 0 in the file.

6.2.7 Flow Observation Files

The Flow Observation dialog box uses the following three formats for saving and loading data. The formats are described in the following sections.

- **Cell Group (∗.cell_group)** contains the data of the Cell Group table of the Flow Observation dialog box (2.75).
- **Flow Observations Data (∗.Flow_observations)** contains observation times, observed values and weights of a cell group. Using the Flow Observation dialog box, a Flow Observations Data file can be loaded to associate with a cell group at a time.
- **Complete Information (∗.complete_flow_obs)** contains all cell groups and their observation data.

6.2.7.1 Cell Group File

```
1. Data: NCELLGROUPS
```

(The following data repeat for each cell group (i.e. NCELLGROUPS times))

```
2. Data: OBSNAM GroupNumber Active Description
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

– **NCELLGROUPS** is the number of cell groups.
– **OBSNAM** is the name of the cell group, max 8 characters, blank and special characters are not allowed
– **GroupNumber** is the number associated with the cell group.
– **Active**: A cell group is active if Active = 1; A cell group is inactive if Active = 0.
– **Description**: Description of the cell group.

6.2.7.2 Flow Observations Data File

```
1. Data: NFOBS
```

(The following data repeat for each observation (i.e. NFOBS times))

```
2. Data: Time, FOBS, STWT
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

– **NFOBS**: number of flow observations
– **Time**: Observation time.
– **FOBS**: observed value at Time.
– **STWT**: STWT is the statistic value for the observation.

6.2.7.3 Complete Information File

```
1. Data: PMWIN6000_FLOW_OBSERVATION
2. Data: NCELLGROUPS EVF
3. Data: Reserved Reserved Reserved Reserved Reserved
4. Data: STAT_FLAG
5. Data: Reserved Reserved Reserved Reserved
```

(The following data repeat for each cell group (i.e. NCELLGROUPS times))

```
6. Data: OBSNAM GroupNumber Active NFOBS
7. Data: Description
```

(The following data repeat NHOBS times for each cell group)

```
8. Data: Time, FOBS, statistic, Reserved
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

- The text string PMWIN_OBSERVATION_FILE must be entered literally.
- **NCELLGROUPS** is the number of cell groups.
- **EVF**: default = 1.
- **STAT_FLAG**: default = 0.
- **OBSNAM**: is the name of the cell group, max 8 characters, blank and special characters are not allowed
- **GroupNumber** is the unique group number associated with the cell group.
- **Active**: A cell group is active if Active = 1; A cell group is inactive if Active = 0.
- **Description**: Description of the cell group.
- **NFOBS**: number of flow observations of a cell group
- **Time**: observation time.
- **FOBS**: observed value at Time.
- **Statistic**: statistic value for the observation.
- **Reserved**: reserved for future use. Enter 0 in the file.

6.2.8 Trace File

A Trace file can be saved or loaded by the Search and Modify dialog box (see Section 2.8.5).

```
File Format
1. Data: LABEL
```

(The following data repeats 50 times, one record for each search range)

```
2. Data: ACTIVE COLOR MIN MAX VALUE OPTION
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

– **LABEL** is the file label. It must be PMWIN_TRACEFILE.

– **ACTIVE** Set ACTIVE = -1 to activate a search range (see MIN / MAX below).

– **COLOR** is the fill color. The color is defined by a long integer using the equation: color = red + green 256 + blue 65536, where red, green and blue are the color components ranging from 0 to 255. COLOR is assigned to the finite-difference cells that have a value located within the search range (see MIN / MAX below).

– **MIN / MAX** define the lower limit and upper limit of the search range.

– **VALUE** According to OPTION (see below), you can easily modify the cell values.
– **OPTION** defines the actions.
OPTION = 0, Display only.
OPTION = 1, Replace: The cell values are replaced by VALUE.
OPTION = 2, Add: VALUE is added to the cell values.
OPTION = 3, Multiply: The cell values are multiplied by VALUE.

6.2.9 Polygon File

A polygon file can be saved or loaded by the Data Editor by selecting *Value* | *Polygon*.

```
File Format
1. Data: LABEL
2. Data: NZONES, XXX, XXX, XXX, XXX
```

(Data 3-6 repeat NZONES times)

```
3. Data: NP
4. Data: PARNO
5. Data: Value(1) Value(2) Value(3) ... Value(I) ... Value(16)
```

(The following data repeats NP times)

```
6. Data: X(J), Y(J)
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

- **LABEL** is the file label. It must be PMWIN4000_ASCII_ZONEFILE or PMWIN_ASCII_POLYGONFILE.
- **NZONES** is the number of polygons. Maximum is 20.
- **XXX** reserved.
- **NP** is the number of vertices of each polygon. The first and the last vertices must overlap. The maximum number of NP is 41.
- **PARNO** is the parameter number (see Sections 2.6.7, 2.6.8 for how to define an estimated parameter).
- **Value(I)** I = 1 to 16; Value(I) are the polygon values. For aquifer parameters, such as porosity or transmissivity, only the first value (or two values, if a parameter number can be defined) is used. For MODFLOW packages, such as Drain Package, as many values as required by the package are used. For example, two values (Hydraulic conductance and the elevation of the drain) required for defining a drain will be saved in Value(1) and Value(2). Other values that are not used must be specified as zero. Table 6.1 gives the assignment of the parameters in the Value(I) vector.
- **X(J),Y(J)** are the (x,y) coordinates of the J-th vertex of the polygon. The first and the last vertices must overlap.

Table 6.1 Assignment of parameters in the Value(I) vector

Package	Value(1)	Value(2)	Value(3)	Value(4)
WEL	Recharge rate	XXX	XXX	XXX
DRN	Hydraulic conductance	Elevation	XXX	XXX
RIV	Hydraulic conductance	Head in river	Elevation	XXX
EVT	Max. ET rate	ET Surface	Extinction Depth	Layer Indicator
GHB	Hydraulic conductance	Head at boundary	XXX	XXX
RCH	Recharge Flux	Layer Indicator	XXX	XXX
HFB	Barrier Direction	K/Thickness	XXX	XXX
IBS	Preconsolidation head	Elastic storage	Inelastic storage	Starting compaction
CHD	Flag	Start head	End head	XXX

The values used by the STR1 package are
Value(1) = Segment; Value(2) = Reach; Value(3) = Streamflow; Value(4) = Stream stage;
Value(5) = Hydraulic conductance; Value(6) = Elevation of the streambed top;
Value(7) = Elevation of the streambed bottom; Value(8) = Stream width;
Value(9) = Stream slope; Value(10) = n/C (Manning's roughness coefficient divided by C).

6.2.10 XYZ File

An XYZ file must be saved as ASCII text using the following format:

N
$X_1\ Y_1\ Z_1$
$X_2\ Y_2\ Z_2$
$\vdots$
$X_i\ Y_i\ Z_i$
$\vdots$
$X_N\ Y_N\ Z_N$

Where N is the number of points; X_i and Y_i are the x, y coordinate values; and Z_i is the data value associated with the point i. All values are are separated by at least one space.

6.2.11 Pathline File

6.2.11.1 PMPATH Format

A pathline file in the PMPATH format is a text file that begins with the header of the form:

@ [PMPATH Version 6.00]

The user may add any number of comment lines following the header line and before the particle data records. Comment lines must contain the "@" symbol in column 1. Comment lines may not be interspersed with the particle data records. The header and comment lines are followed by a sequence of lines. Each line contains the following data items in the order specified:

1. Particle index number. The index number is positive, if the forward particle-tracking scheme is used. A negative index number indicates that the backward particle-tracking scheme is used.
2. Global coordinate in the x-direction.
3. Global coordinate in the y-direction.
4. Local coordinate in the z-direction within the cell.
5. Global coordinate in the z-direction.
6. Cumulative tracking time.
7. J index of cell containing the point.
8. I index of cell containing the point.
9. K index of cell containing the point.
10. RGB-Color of the pathline.

6.2.11.2 MODPATH Format

The standard text pathline file of MODPATH (Pollock [93][95]) is a text file that begins with the header of the form:

@ [MODPATH Version 3.00 (V3, Release 1, 9-94) (TREF= 0.000000E+00)]

The user may add any number of comment lines following the header line and before the particle data records. Comment lines must contain the "@"symbol in column 1. Comment lines may not be interspersed with the particle data records.

The header and comment lines are followed by a sequence lines. Each line contains the following data items in the order specified:

1. Particle index number
2. Global coordinate in the x-direction
3. Global coordinate in the y-direction
4. Local coordinate in the z-direction within the cell
5. Global coordinate in the z-direction
6. Cumulative tracking time
7. J index of cell containing the point
8. I index of cell containing the point
9. K index of cell containing the point
10. Cumulative MODFLOW time step number

6.2.12 Particles File

A Particles File is a a text file that begins with the header of the form:

```
1. Data:  PMPATH_V100_PARTICLES
2. Data:  NP
```

(The following data repeats NP times)

```
3. Data:  LI  LJ  LK  I  J  K  Z  C  R
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

– The text string *PMPATH_V100_PARTICLES* must be entered literally.
– **NP** is the number of particles.
– **LI**: Local coordinate in the row direction
– **LJ**: Local coordinate in the column direction
– **LK**: Local coordinate in the layer direction
– **I**: Row index of cell containing the particle
– **J**: Column index of cell containing the particle

– **K**: Layer index of cell containing the particle
– **Z**: global vertical coordinate of the particle
– **C**: Color of the particle
– **R**: Retardation factor associated with the particle

The particle locations within the cell [J, I, K] are specified using local coordinates [LJ, LI, LK]. Local coordinates vary within a cell from zero to one as shown in Fig. 6.1.

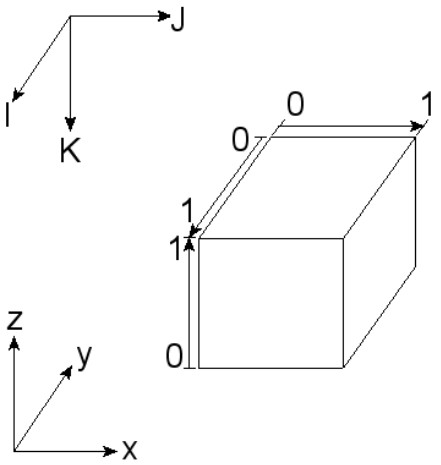


Fig. 6.1. Local coordinates within a cell

6.3 Input Data Files of the supported Model

6.3.1 Name File

The name file contains the names of most input and output files used in a model simulation and controls the parts of the model program that are active. The format of the name file for MODFLOW 88/96 is identical to that of MODFLOW-2000, except the latter has some additional file types marked with the * character (see Ftype below). The name file contains one record similar to the following line for each input and output file used in a MODFLOW model simulation. All variables are free format. The length of each record must be 199 characters or less.

```
Ftype    Nunit    Fname
```

Explanation of Fields Used in Input Instructions

All data in the same record are separated by at least one space.

- **Ftype** is the file type, which must be one of the following character values. Ftype may be entered in all uppercase, all lowercase, or mixed case.
  - **LIST** for the simulation listing file.
  - **BAS** for the Basic Package of MODFLOW.
  - **BCF** for the Block-Centered Flow Package of MODFLOW.
  - **CHD** for the Time-Variant Specified-Head Package.
  - **DE4** for the Direct Solver Package
  - **DRN** for the Drain Package.
  - **EVT** for the Evapotranspiration Package
  - **HFB** for the Horizontal Flow Barrier Package of MODFLOW.
  - **GHB** for the General-Head Boundary Package.
  - **IBS** for the Interbed Storage package
  - **OC** for the Output Control Option
  - **PCG** for the Preconditioned Conjugate Gradient 2 Package
  - **RCH** for the Recharge Package
  - **RIV** for the River Package.
  - **SIP** for the Strongly Implicit Procedure Package
  - **SOR** for the Slice-Successive Over-Relaxation Package
  - **STR** for the Streamflow Routing Package.
  - **WEL** for the Well Package.
  - **DIS*** for the discretization file.
  - **BAS6*** for the Basic Package of MODFLOW-2000.
  - **BCF6*** for the Block-Centered Flow Package of MODFLOW-2000/-2005.
  - **LPF*** for the Layer Property Flow package of MODFLOW-2000/-2005.
  - **HFB6*** for the Horizontal Flow Barrier Package of MODFLOW-2000/-2005.
  - **LMG*** for the Link Algebraic Multigrid Solver Package of MODFLOW-2000/-2005.
  - **OBS*** for the main input file to the Observation Process of MODFLOW-2000.
  - **HOB*** for the Head Observation Package of MODFLOW-2000.
  - **DROB*** contains the observed flows to features represented by the Drain package. This file is used by the Observation Process of MODFLOW-2000.
  - **GBOB*** contains the observed flows to features represented by the General-Head Boundary package. This file is used by the Observation Process of MODFLOW-2000.
  - **RVOB*** contains the observed flows to features represented by the River package. This file is used by the Observation Process of MODFLOW-2000.
  - **STOB*** contains the observed flows to features represented by the Streamflow-Routing package. This file is used by the Observation Process of MODFLOW-2000.
  - **CHOB*** contains the observed flows to features represented by the Time-Variant Specified-Head package. This file is used by the Observation Process of MODFLOW-2000.
  - **SEN*** for the Sensitivity Process of MODFLOW-2000.
  - **PES*** for the Parameter Estimation Process of MODFLOW-2000.

  - **ZONE*** for the Zone Array file of MODFLOW-2000.
  - **MULT*** for the Multiplier Array file of MODFLOW-2000.
  - **DATA(BINARY)** for binary (unformatted) files such as those used to save cell-by-cell budget data and binary (unformatted) head and drawdown data.
  - **DATA** for formatted (text) files, such as those used for input of data from files that are separate from the primary package input files.
- **Nunit** is the Fortran unit to be used when reading from or writing to the file. Any legal unit number on the computer being used can be specified except units 96-99.
- **Fname** is the name of the file. The path names may be specified as part of Fname.

Example of a Name File

```
LIST 6 output.dat
BAS 1 bas.dat
BCF 11 bcf.dat
OC 22 oc.dat
WEL 12 wel.dat
RCH 18 rch.dat
PCG 23 pcg2.dat
DATA(BINARY) 50 budget.dat
DATA(BINARY) 51 heads.dat
DATA(BINARY) 52 ddown.dat
DATA(BINARY) 32 mt3d.flo
```

6.3.2 MODFLOW-96

Basic Package	BAS.DAT
Block-Centered Flow Package	BCF.DAT
Density Package (DEN1)	DEN1.DAT
Direct Solution Package (DE45)	DE45.DAT
Drain Package	DRN.DAT
Evapotranspiration Package	EVT.DAT
General-Head Boundary Package	GHB.DAT
Horizontal-Flow Barrier Package	HFB1.DAT
Interbed-Storage Package	IBS1.DAT
Output Control	OC.DAT
Preconditioned Conjugate Gradient 2 Package (PCG2)	PCG2.DAT
River Package	RIV.DAT
Recharge Package	RCH.DAT
Reservoir Package	RES1.DAT
Strongly Implicit Procedure Package	SIP.DAT
Slice-Successive Overrelaxation Package	SOR.DAT
Stream-Routing Flow Package	STR1.DAT
Time Variant Specified Head	CHD1.DAT
Well Package	WEL.DAT

6.3.3 MODFLOW-2000/-2005

Discretization File	DISCRET.DAT
Basic Package	BAS6.DAT
Zone Array File	ZONE.DAT
Multiplier Array File	MULTIPLE.DAT
Layer-Property Flow Package	LPF6.DAT
Block-Centered Flow Package	BCF6.DAT
Drain Package	DRN6.DAT
Evapotranspiration Package	EVT6.DAT
General-Head Boundary Package	GHB6.DAT
Horizontal-Flow Barrier Package	HFB6.DAT
Interbed-Storage Package	IBS1.DAT
Recharge Package	RCH6.DAT
Stream-Routing Flow Package	STR6.DAT
Reservoir Package	RES1.DAT
River Package	RIV6.DAT
Time Variant Specified Head	CHD6.DAT
Well Package	WEL6.DAT
Strongly Implicit Procedure Package	SIP.DAT
Slice-Successive Overrelaxation Package	SOR.DAT
Direct Solution Package (DE45)	DE45.DAT
Link Algebraic Multigrid Solver Package	LMG.DAT
Preconditioned Conjugate Gradient 2 Package (PCG2)	PCG2.DAT
Output Control	OC.DAT
Observation Process	OBS_MAIN.DAT
Sensitivity Process	SEN.DAT
Parameter Estimation Process	PES.DAT
Head Observation Package	HOB.DAT
Observed flows to features represented by the Drain package	DROB.DAT
Observed flows to features represented by the General-Head Boundary package	GBOB.DAT
Observed flows to features represented by the River package	RVOB.DAT
Observed flows to features represented by the Streamflow-Routing package	STOB.DAT
Observed flows to features represented by the Time-Variant Specified-Head package	CHOB.DAT

6.3.4 MODPATH and MODPATH-PLOT (version 1.x)

Main data file	MAIN.DAT

(Other files required by MODPATH, such as RIV.DAT or WEL.DAT are the same as those of MODFLOW 88/96.)

6.3.5 MODPATH and MODPATH-PLOT (version 3.x)

Main data file	MAIN30.DAT

(Other files required by MODPATH, such as RIV.DAT or WEL.DAT are the same as those of MODFLOW 88/96.)

6.3.6 MOC3D

Main MOC3D Package	MOCMAIN.DAT
Source Concentration in Recharge	MOCCRCH.DAT
Observation Well File	MOCOBS.DAT

(Other files required by the flow simulation, such as RIV.DAT or WEL.DAT are the same as those of MODFLOW 88/96.)

6.3.7 MT3D

Advection Package	MTADV1.DAT
Basic Transport Package	MTBTN1.DAT
Chemical Reaction Package	MTRCT1.DAT
Dispersion Package	MTDSP1.DAT
Sink & Source Mixing Package	MTSSM1.DAT

6.3.8 MT3DMS/SEAWAT

Advection Package	MTMSADV1.DAT
Basic Transport Package	MTMSBTN1.DAT
Chemical Reaction Package	MTMSRCT1.DAT
Dispersion Package	MTMSDSP1.DAT
Generalized Conjugate Gradient Solver	MSMSGSG1.DAT
Sink & Source Mixing Package	MTMSSSM1.DAT
Variable Density Flow Package (SEAWAT Only)	SW2KVDF1.dat

6.3.9 RT3D

Advection Package	MTMSADV1.DAT
Basic Transport Package	MTMSBTN1.DAT
Chemical Reaction Package	MTMSRCT1.DAT
Dispersion Package	MTMSDSP1.DAT
Generalized Conjugate Gradient Solver	MSMSGSG1.DAT
Sink & Source Mixing Package	MTMSSSM1.DAT

6.3.10 PHT3D

Advection Package	PHT3DADV.DAT
Basic Transport Package	PHT3DBTN.DAT
Chemical Reaction Package	PHT3DRCT.DAT
Dispersion Package	PHT3DDSP.DAT
Generalized Conjugate Gradient Solver	PHT3DGCG.DAT
Sink & Source Mixing Package	PHT3DSSM.DAT
PHREEQC Interface File	PHT3D_PH.DAT
PHREEQC-Style Database File	PHT3D_DATAB.DAT

6.3.11 PEST

Instruction File	INSTRUCT.DAT
Control File	PESTCTL.DAT
Block-Centered Flow Package Template File	BCFTPL.DAT
Drain Package Template File	DRNTPL.DAT
Evapotranspiration Package Template File	EVTTPL.DAT
General-Head Boundary Package Template File	GHBTPL.DAT
Recharge Package Template File	RCHTPL.DAT
River Package Template File	RIVTPL.DAT
Well Package Template File	WELTPL.DAT
Stream-Routing Flow Package Template File	STRTPL.DAT
Interbed-Storage Package Template File	IBSTPL.DAT
Grid Specification File (used by MODBORE.EXE)	*filename*.GRD*
Borehole Listing File (used by MODBORE.EXE)	BORELIST.DAT
Borehole Coordinates File (used by MODBORE.EXE)	BORECOOR.DAT

* *filename* is the name of the model.

6.4 Using MODPATH with PM

PM supports two versions (version 1.x and 3.x) of MODPATH and MODPATH-PLOT. Since MODPATH and MODPATH-PLOT reads the binary model result files from MODFLOW, these programs needed to be compiled with the same Fortran-Compiler to ensure the binary compatibility between them. The MODFLOW programs, which come with pmp, are compiled with Lahey-Fortran 95. To run MODPATH or MODPATH-PLOT with **PM**, these programs need to be compiled the same compiler too. The users can, however, use their own compiler to compile the MODFLOW, MODPATH and MODPATH-PLOT for using with pmp. See Section 1.2 for details.

MODPATH or MODPATH-PLOT must be started within a DOS-Box (of Windows) or in the DOS-Environment.

When using MODPATH version 1.x (released prior to September, 1994), type path\PATHFILE at the prompt ENTER NAME OF FILE CONTAINING NAMES AND UNITS OF DATA FILES. Where path is the path to the directory of your model data. PATHFILE contains the IUNIT assignments and paths and names of input data files generated by PMWIN. The names of the input files for MODFLOW and MODPATH are given in Sections 6.3.2, 6.3.4, and 6.3.5.

When using MODPATH or MODPATH-PLOT (version 3.x), follow the steps below:

TO READ INPUT FROM AN EXISTING RESPONSE FILE, ENTER FILE NAME:
(<CR> = ENTER DATA INTERACTIVELY)
[? = Help]

(WHAT TO DO: Just press ENTER here. When running MODPATH or MODPATH-PLOT at the first time, a response file does not exist and the user has to enter data interactively. The user-specified data will be saved by MODPATH or MODPATH-PLOT in the response files MPATH.RSP or MPLOT.RSP, respectively. Using a response file, it is not necessary to go through the input procedures unless the data for MODPATH or MODPATH-PLOT need to be changed).

Only for MODPATH-PLOT:

TO REDEFINE SETTINGS, ENTER NAME OF FILE WITH SETTINGS DATA:
(<CR> = USE DEFAULT SETTINGS FOR DEVICE)
[? = Help]

(WHAT TO DO: Just press ENTER here, unless the settings need to be changed.)

ENTER THE NAME FILE:
[? = Help]

(WHAT TO DO: Type *path*\MPATH30 at this prompt. Where *path* is the path to the directory of your model data. For example, if model data are saved in C:\PMWIN\DATA, type C:\PMWIN\DATA\MPATH30 at this prompt. After this prompt, the user enters the interactive input procedure of MODPATH or MODPATH-PLOT. Just follow the prompts of the programs.)

6.5 Define PHT3D Reaction Module

Before creating a *new* user-defined reaction module, a basic knowledge of PHREEQC-2 must be obtained and, at least for more complex cases, it is strongly recommended to first test and debug reaction definitions in batch-mode, i.e., by setting up a PHREEQC-2 batch-type simulation. To add a user-defined PHT3D reaction module for **PM**, you need to complete the following three steps:

1. Create a database file analogous to the original PHREEQC-2 database files. You can find a number of examples, such as *pht3d_datab.ex1*, *pht3d_datab.ex2*, etc., in the *pmdir/pht3d/Database* folder, where *pmdir* is the installation folder of **PM**.
2. Create a module file that contains information about the number, names and types of chemical, and reaction rate constants that are used in the corresponding database file created in the first step. You can find a number of examples and templates in the */pht3d/Database*. For example, pmwin_pht3dv2.standard contains information corresponding to the standard PHREEQC-2 database file pht3d_datab.standard.
3. Add module definition to the *pmdir/pht3d/Database/pht3d_module_definition.txt* file. To add a module definition, you need to modify the number of modules in the *pht3d_module_definition.txt* file, and then add the four lines containing the following information to the end of the *pht3d_module_definition.txt* file:
   - *Name of the module*
   - *Description of the module*
   - *Name of the PHREEQC database file created in step 1.*
   - *Name of the module file created in step 2*

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